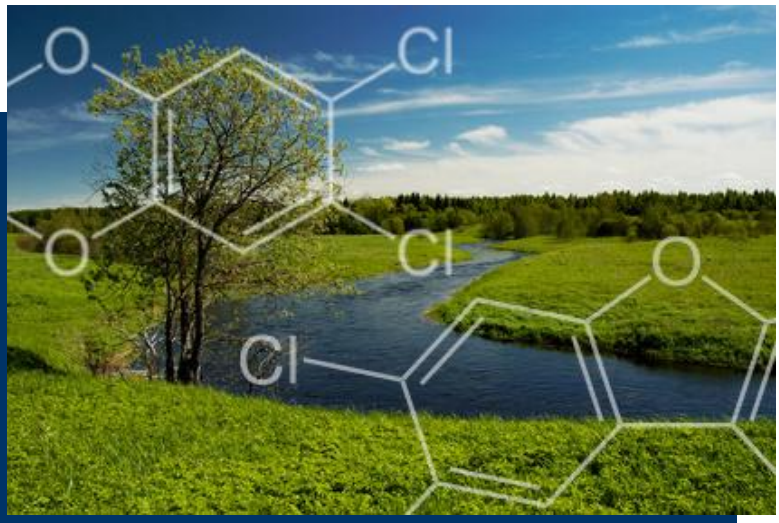
User Manual
POP-Dioxin Search Application



POPD
Search Application
POP-Dioxin Database

Target group: Users
POPD Version: 1

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1 About this document

This “User Manual” describes the design and interaction of the software modules making up the “POP-Dioxin Search Application”. It is organized on the principle of working from the general to the particular.

The User Manual describes the solutions designed and implemented for the UBA from the point of view of the user. It also considers technical aspects where this is necessary for better understanding.

A separate section first gives the reader an overview of the basic concepts for using the application, and of the system architecture. The following sections then give a detailed description of the modules that interact within the architecture described.

1.1 Basis for solution

The basis for the solution is the invitation to tender for the “development of the new POP-Dioxin Database web service” and the order placed by the Federal Environment Agency (UBA) in response to the bid by Condat AG.

1.2 The module concept

Module: A module provides a set of functions that cover a specific spectrum of tasks. For example, a module may be a group of screens that are all used to perform a certain technical task. A module may also provide functions grouped by technical criteria.

Interface: A module offers external interfaces. These may be user interfaces or program interfaces. Program interfaces are accessed by other modules or from within other modules. This document regards user interfaces and program interfaces as equally important.

Function: A functionality that can be called or run via an interface. Synonym: Feature

1.3 Structure of module descriptions

Each module is described in a separate chapter. The structure of these chapters is always the same:

- an introductory text,
- the description of the interfaces,
- the functions, and
- the data model (optional)

2 Overview

Thanks to its great flexibility and ease of use, the POP-Dioxin Search Application enables users, and especially expert users with no prior technical knowledge, to define and perform searches geared to a specific information need and to share them with other users. The POP-Dioxin Search Application permits:

1. **Selection:** targeted and flexible selection of environmental data from the Federal and Länder dioxin database,
2. **Analysis:** analysis and aggregation of the selected environmental data, and their
3. **Presentation:** informative and meaningful presentation of the results of selection and/or analysis.

Thus the overall system "POP-Dioxin Search Application" consists of the basic modules corresponding to the steps **"Selection"**, **"Analysis"** and **"Presentation"** (see below).

The functions of these modules are integrated by the application framework (see below).

2.1 Technical basis

The solution developed by Condat uses a software architecture that is rigorously based on modules with functionality provided by clearly defined module interfaces. In particular, the high degree of modularity makes the system very easy to maintain. The basis for this is clear separation of the various levels of implementation:

1. The lowest level, the **basic level** of all modules in the POP-Dioxin Search Application, consist of robust and widespread basic frameworks. These include in particular Java 1.6, Eclipse Rich Client Platform (RCP), Eclipse Rich Ajax Platform (RAP) and Hibernate.

2. On top of the **basic level**, the next level creates a pool of **OSGi[1] components**.

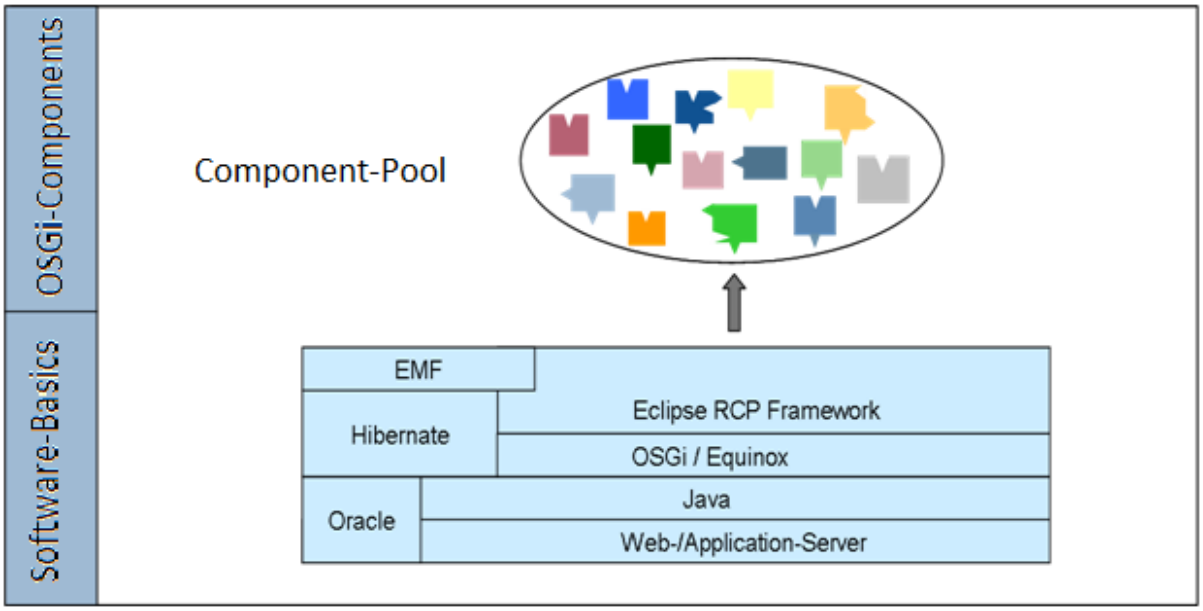


Figure 1: Component pool

[1] OSGi: Open Services Gateway initiative

3. The modules of the POP-Dioxin Search Application are themselves made up of **OSGI components**. The modules are integrated to form the “POP-Dioxin Search Application”. To this end the functions of the suitably configured modules are called from the **application framework** of the “POP-Dioxin Search Application”.

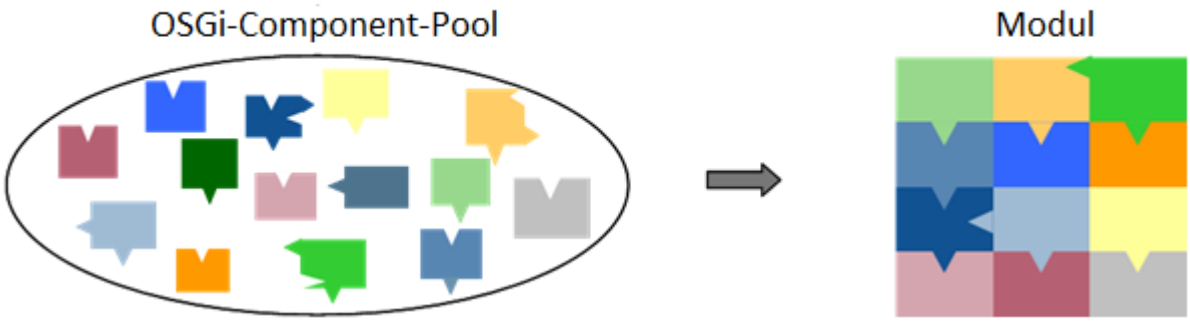


Figure 2: Modular composition

Basic level

Condat AG's concept for the POP-Dioxin Search Application described here is based on rigorous use of Eclipse technologies. Eclipse is an open source community whose projects aim to create an open software development platform. This platform consists of extensible frameworks, tools and runtime components for building and implementing software products and for deploying and managing the resulting software over its entire life cycle. The functional spectrum of the frameworks is enormous. It includes components for the development of modern web applications, service-oriented architectures or classic J2EE systems. Powerful tools for diagrams and reporting, model-based development and data access are already integrated.
The great stability of the POP-Dioxin Search Application is achieved by making exclusive use of mature, tried-and-tested and widely used open source software backed up by a powerful developer community. The basic software, for which great developer potential exists, is continuously developed and improved by the relevant communities (many of whom are employees of companies such as IBM and SAP).

OSGi components

The POP-Dioxin Search Application consists of modules which are in turn made up of OSGi components. The fully developed open-source OSGi implementation "Equinox" from the Eclipse project is used as the OSGi framework.

An important aspect for the development of the POP-Dioxin Search Application is the fact that the use of OSGi components greatly encourages a development style known as Component Oriented Development and Assembly (CODA), which aims from the outset to develop applications on the basis of modules.

OSGi components can be integrated in services and applications without making any changes in their implementation. Depending on the runtime environment, they can even be added, removed or replaced while an application is running.

Third-party software that is not already available as an OSGi component can be encapsulated as an OSGi component, making it possible to access functions exclusively via the OSGi component interfaces.

The greatest advantage of the component model described is that very close coupling and hence high performance at runtime is guaranteed despite the approach of loose coupling of software components (high degree of encapsulation, declarative interfaces, configurability, hot deployment).

The advantages of using OSGi components within the POP-Dioxin Search Application are:

- Supports the modular structure of the application
- Flexible combination of components for different types of application and target groups

The OSGI components of the POP-Dioxin Search Application are executed using the "Java" programming language with the aid of the basic level framework.

Modules

The modules used in the POP-Dioxin Search Application are implemented on the basis of the OSGi components. The application framework serves to integrate the functionality provided by the modules.

2.2 Three-layer software architecture

The modules of the POP-Dioxin Search Application are all based on the same structure:

1. **Control**: The application interfaces are implemented using the standard resources of the Eclipse-RCP platform, with Eclipse RAP being used to make the web application available.
2. **Technical functions** (logic level): Implementation is solely in Java on the basis of the Eclipse-RCP platform.
3. **Data storage**: Here the Eclipse Modelling Framework (EMF) is used to represent the domain and helper objects in Java, and Hibernate to store the data in the ORACLE database.

The three layers “Control”, “Expert functions” and “Data storage” are kept strictly separate and are implemented in separate OSGi components (if necessary more than one per level, depending on expert/technical needs).

Basic modules

Focusing on the “Control” and “Expert functions” layers, the following description provides an insight into the interactions between the modules in the POP-Dioxin Search Application.

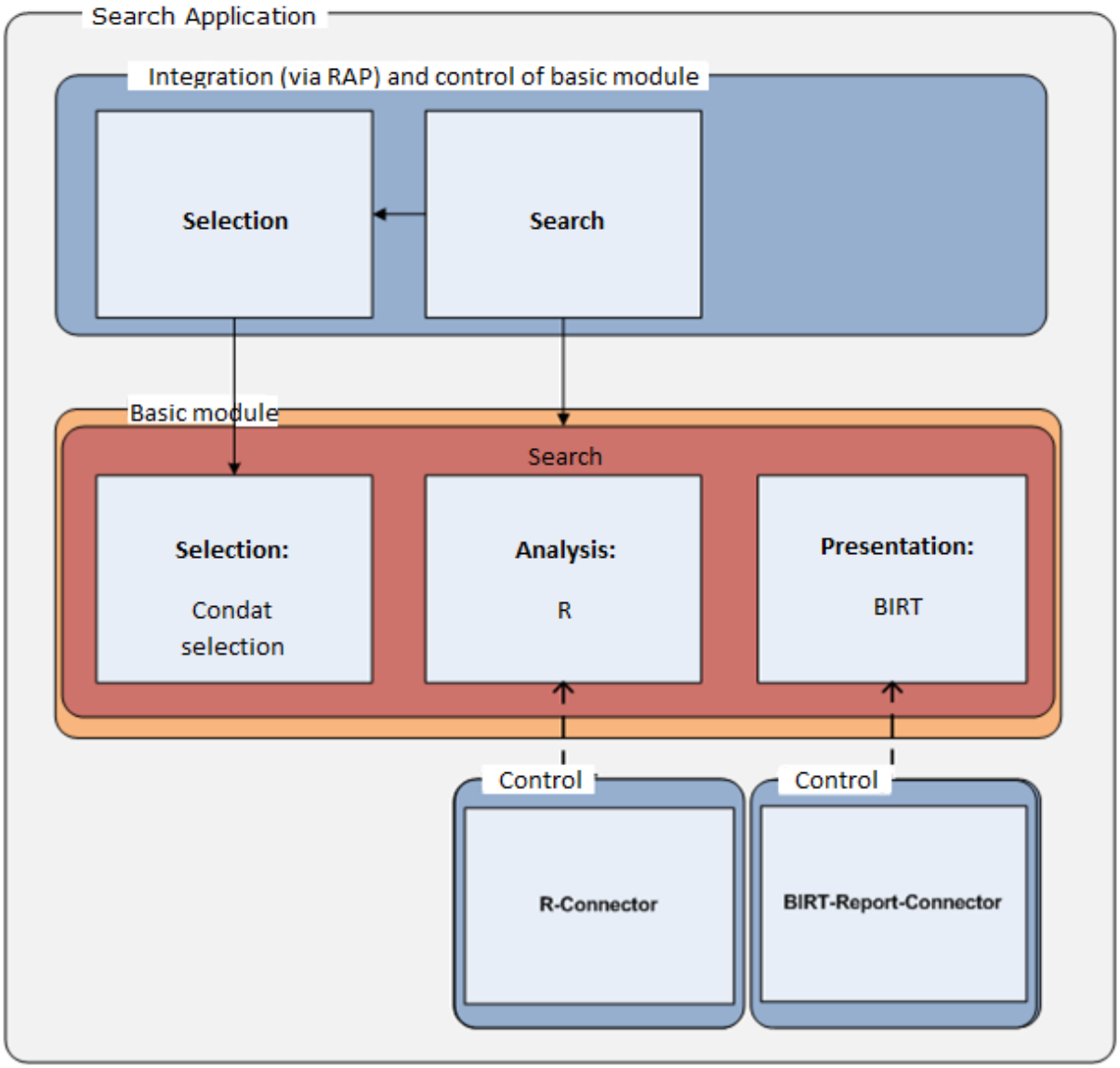


Figure 3: Overview of architecture

The modules **“Selection”**, **“Analysis”**, **“Presentation”** and **“Search”** form the basic modules for the POP-Dioxin Search Application.

Selection: The extended Condat selection component is used as the selection module. The Condat selection component was developed as part of the “IMIS” and “PKS” projects. Its most important feature is the reference to the scientific model, which ensures a specialized configuration for the relevant expert domain and makes its use intuitive and easy to learn for the expert user.

Analysis: The integration of the open-source statistical software R (R Foundation) makes it possible to use statistical methods to analyze previously selected data. R is integrated in the otherwise Java-based Eclipse world by means of the Java libraries provided for this purpose by the company

"Revolution Analytics". The integration of R using "Revolution Analytics" products is effected in a way that enables expert users to employ scripts of their own to extend the functionality of the statistics module. This allows the existing wealth of experience of expert users to be transferred into the POP-Dioxin Search Application.

Presentation: The diagrams needed for presenting the selection results and the statistical analysis are provided by the open-source reporting system "BIRT" for web applications (Eclipse Foundation).

Search: The Search module coordinates the interaction of **Selection**, **Analysis** and **Presentation**.

Integration and control

The control elements that enable the user to interact with the basic modules in order to make use of their expert functions (logic level) are integrated by means of the application framework of the "POP-Dioxin Search Application". There the control elements are embedded in a uniformly designed user interface in the interest of maximizing ergonomics and hence operating reliability.

In addition to the POP-Dioxin Search Application, the overall system also includes the separate desktop applications "BIRT Report Designer" and "RevoDeployR", which are used for independent definition of BIRT reports and R analysis scripts. Once they are completely defined, the BIRT reports and R analysis scripts are made available to the runtime environment of the POP-Dioxin Search Application with the aid of the "BIRT Report Connector" and "R-Connector". R analysis scripts and BIRT reports (diagrams) are then available for access by the users of the POP-Dioxin Search Application.

3 Application framework of the search application

3.1 Description of the module

Application framework

The application framework forms the infrastructure of the search application. The application framework brings together the functionality of the modules "Search", "Selection", "Analysis" and "Presentation". The module "Rights" also plays an important role. The "Rights" module provides standardized mechanisms for authorization checking.

All these modules presented in more detail in this solution concept and the application framework itself are based on the same concepts and basic frameworks (see 2.1 Technical basis). This ensures both a standardized software structure and standardized operation of the search application.

The application framework offers two user views of the POP-Dioxin Search Application:

- Search
- Administration

The "Search" view is used to compose searches and perform the composed searches.

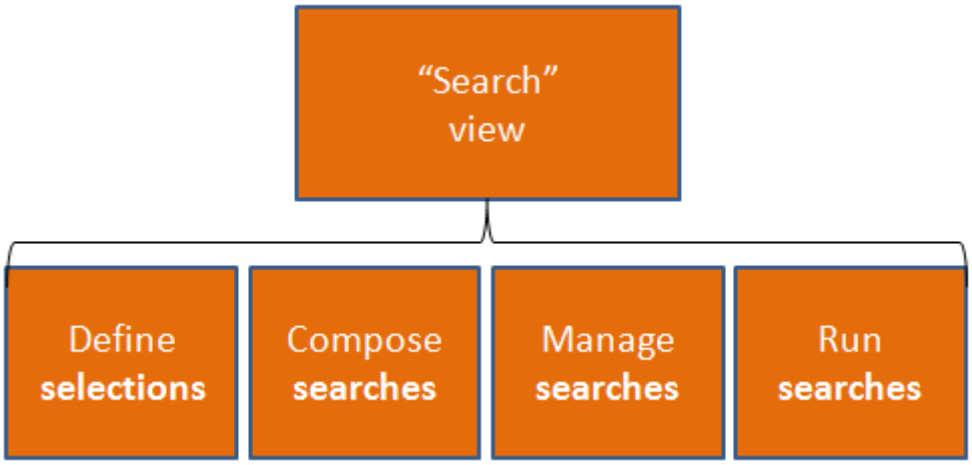


Figure 4: "Search" view

The analysis definitions and presentation definitions needed for composing a search are registered with the search application in a separate area of the application, using the "Administration" view. This is also used for user administration purposes.

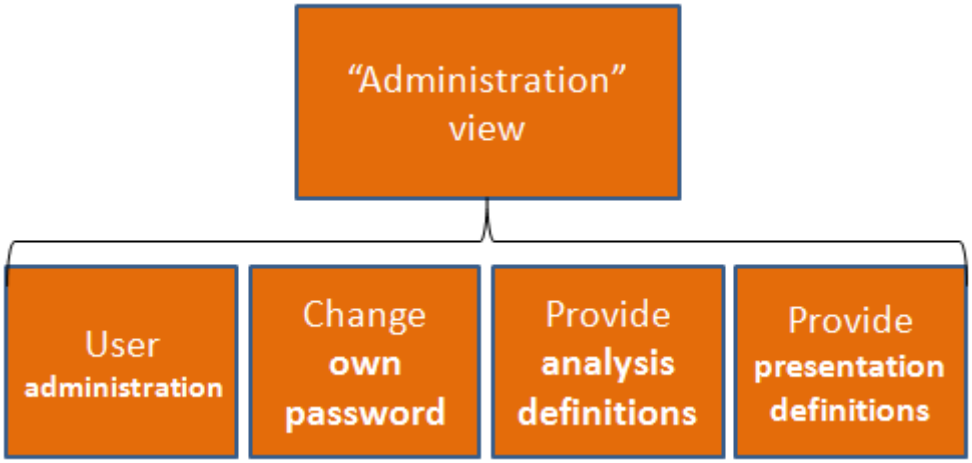


Figure 5: "Administration" view

Two-stage use concept

In software development, the requirement of "simple operation combined with great flexibility" often implies an insoluble contradiction:

As a rule, the more flexibility, variability and general functional scope a software product offers, the more complicated it is to operate. When designing the POP-Dioxin Search Application, this conflict was resolved by means of a two-stage use concept:

Stage 1) Expert users define a search and make it available

The POP-Dioxin Search Application helps expert users to define and make available pre-defined searches, and serves as a search development environment for specialists.

Stage 2) All users of the search application run the defined searches provided.

Once made available, the defined searches can be run at any time to obtain an up-to-date result. Specified selection parameters may be changed when running the searches.

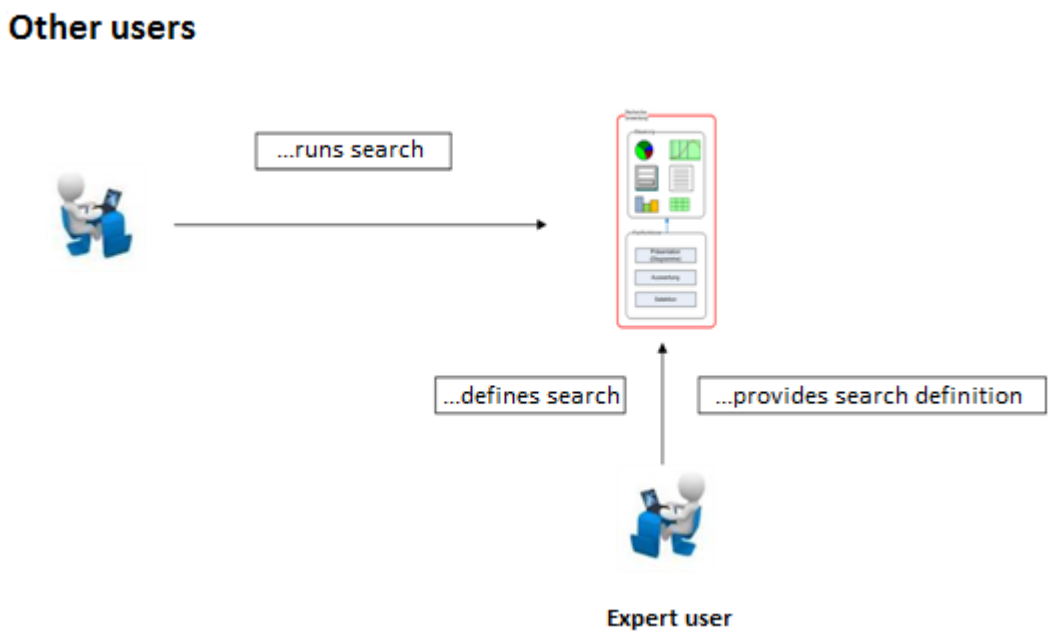


Figure 6: Two-stage use concept

The advantage of this approach lies in the great flexibility when creating searches, combined with subsequent easy operation when performing the searches provided.

The expert users' entire expert knowledge can flow into the definition of the searches and their individual modules "Selection", "Analysis" and "Presentation". The creator of the search can then make it available to other users. Then it is only necessary to run the defined searches to obtain an up-to-date analysis of the data. Thus a user can select and run a search tailored to his specific information needs from the stock of defined searches. This ensures very easy operation without restricting the expert content of the information obtained using the POP-Dioxin Search Application.

It goes without saying that the expert users are free to define their own searches at all times. In principle, users have a great deal of freedom to create and store individual search definitions within their personal sphere.

User interfaces

The POP-Dioxin Search Application is implemented as a web application. The user interface comprises the following building blocks:

- Header area with menu bar
- Navigation pane
- Dialog and work area with editors for entering search criteria, displaying search results etc.

Only interface elements and functions supported by Eclipse-RAP are permitted.

The **menu bar** can be used to select the application views “Search” and “Administration”.

If the “Search” view is selected, the following folders are shown in the **navigation pane**:

- User group specific searches (groups are formed on the basis of expert, not organizational criteria)
- “My searches” (user’s private sphere)

The folder “My searches” (private sphere) can be used to define searches which can subsequently be made available to the other users in the group folders.

3.2 Interfaces

3.2.1 Screens

POPD-294 - Login
Access to the search application is only possible after a successful login. The login process checks the validity of a login name and password combination. The password is encrypted. Blocked users are unable to login.

POPD-333 - UI design
The user interface design is simple and user-friendly. Apart from a menu bar for selecting the application view (see 3.2.1 Views), the application header does not contain any other elements. The Dioxin-DB logo appears on the left side above the menu bar for selecting the view.
Directly below it is the navigation pane, and to the right of this the editor pane.

POPD-295 - Welcome page
A welcome page is shown when the application starts up. The welcome page explains the distinction between free searches and the possibility of using pre-defined searches provided in the technically structured group folders. In addition, the “Standard” group offers standard searches for the user to run.

POPD-169 - Views
Two views of the application are implemented, namely “Search” and “Administration”.
The “Search” view offers the standard functions for composing and performing searches. The

“Administration” view provides the functions for making available analysis definitions and presentation definitions. The administration of user rights (user administration) is also included in this view.

POPD-387 - Navigation pane
A navigation pane is displayed on the left below the application menu. Here a simple tree structure makes it possible to select a domain object for editing or for running a search. The POP-Dioxin Search Application has the following domain objects:

- Searches
- Analysis definitions
- Presentation definitions
- Users

POPD-167 - Editor pane
The editor pane for defining searches and query definitions comprises several **editor pages** which can be freely selected by means of tabs.

As well as free selection of the various editor pages by means of tabs, “Forward” and “Back” buttons are provided for moving to the next or previous editor page. The tab for an editor page belonging to a working step is always marked, showing the user’s current position within the edit workflow. This maps out a standardized edit workflow which nevertheless leaves experts the full variability of free access.
A “Save” button is also provided.

The editor page descriptors used in the “Search” view of the search application have the following syntax:
"<Group> + ": " + <Name> + ": " + <Editor-Typename>
It is not possible to open the same search in more than one editor.

POPD-369 - Error message display
Error messages are displayed in a standardized format.

POPD-347 - Exit application
The application is ended by clicking on the menu item “Logout”, by closing the browser, or in response to a time-out.

4 Search module

4.1 Description of the module

The Search module coordinates the interaction of the activities **“Query”**, **“Analysis”** and **“Presentation”**.

These activities are performed by the sub-modules **“Selection”**, **“Analysis”** and **“Presentation”**, with interim results (query result of analysis result) being passed to the next activity in the sequence.

The metadata items describing these individual activities are termed **“Query definition”**, **“Analysis definition”** and **“Presentation definition”**. In particular, the metadata describe the structure and form of the parameters transferred.

Searches are composed of exactly one query definition, not more than one analysis definition and not more than one presentation definition. In other words, the specification of an analysis definition and a presentation definition is optional.

When a search is performed, the individual activities described by query definition, analysis definition and presentation definition are carried out in sequence.

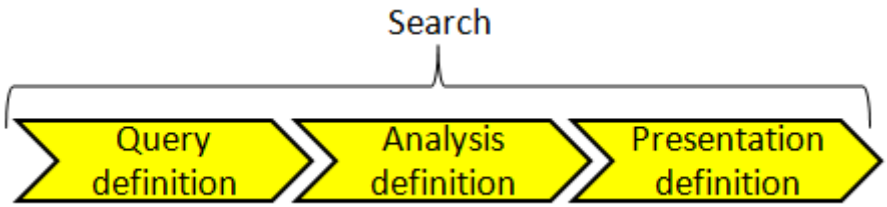


Figure 7: Structure of a search

The sub-modules “Selection”, “Analysis” and “Presentation” supply each other with data in tabular form when queries, analyses and presentations are performed. The selection module hands over the query result (exactly one table) to the analysis module or the presentation module. The analysis module also supplies a tabular representation of the analysis results (also exactly one table) to the presentation module. Accordingly, the presentation module and the analysis module always expect a tabular structure as input.

For this process to function, the expert designing the search must deposit the expected input for each individual activity as metadata. The result of the analyses must also be described.

For queries, the metadata are initially deposited in the data model metadata, so that a user defining a query only needs to make a selection from the pre-configured information.

4.2 Interfaces

4.2.1 Screens

POPD-336 - Search application modes
In line with its two-stage use concept, the POP-Dioxin Search Application distinguishes the two modes “Run” and “Edit”.

The “Edit” mode is for defining searches and offers the user all the features of the application.
The “Run” mode is simpler and is designed so that it always takes the user only a few clicks to obtain a result. In particular, only the search criteria previously defined in Edit mode can be changed. Searches from the group folders can only be opened in Run mode.

POPD-374 - Navigation pane (Search)
The navigation pane for searches is divided into two sections arranged one above the other. In the upper section a folder or node is displayed for each group that the current user belongs to. Below this folder a list of all searches released for this group is displayed without any further substructure. Searches listed in the group folders are not available for editing. They are owned by the group and can no longer be changed once they have been released. This ensures that released searches always provide the group members with the expected results.

A section for “My searches” is provided below the group folder section for the user to define new searches and edit existing ones. This lists all searches defined by the current user. Searches in the “My searches” section can be freely edited, and new searches can be added. All searches managed here – just like searches from the group folders – can of course be run directly by the current user (action “Run”).

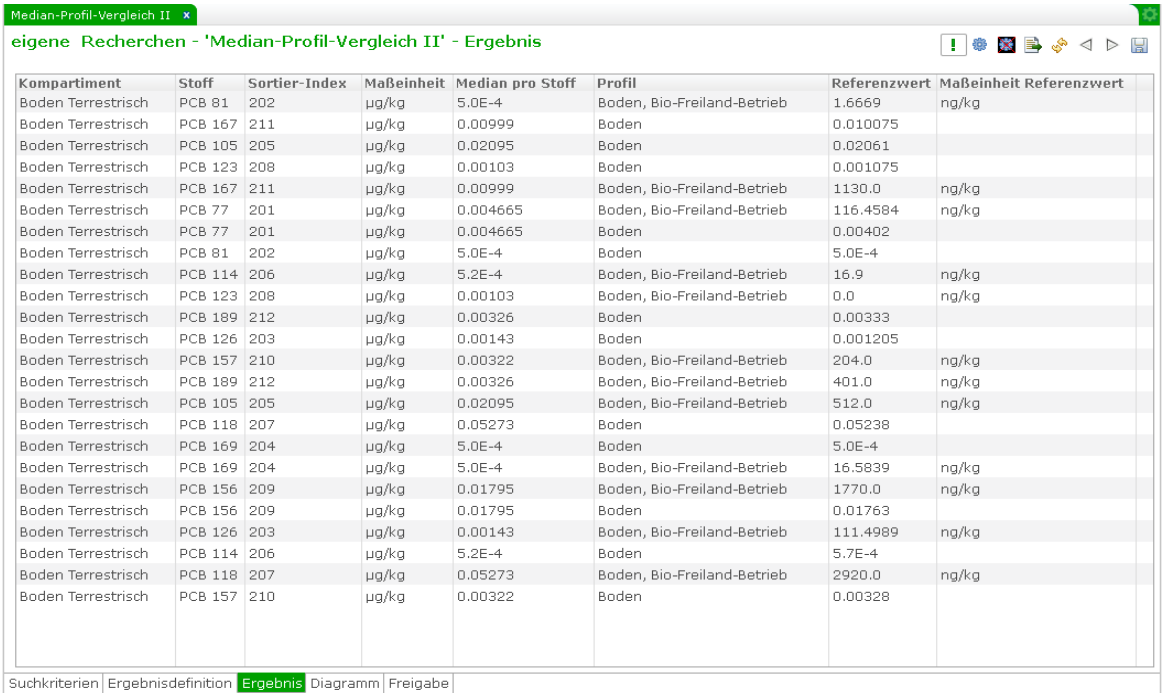
If it is necessary to change a search in one of the group folders, it must first be deleted from the group folder. Then the author of the original search can create and test an existing or new search in his private sphere and finally release it again under the name of the deleted search for use by the desired groups.

POPD-417 - Query (Search and Result Definition)
Defining a query to the underlying database, just like refining and completing a query that has already been defined, is done with the aid of the control elements “Search” and “Result Definition” of the “Selection” module. To this end the control elements “Search” and “Result Definition” (see 6.2.1 Search (Run), 6.2.1 Search (Edit) and 6.2.1 Result Definition) are integrated in the control of the Search module. Depending on the mode in which the relevant search is opened (“Run” or “Edit”), the editor page “Search” is opened with restricted functionality (6.2.1 Search (Run)) or extended functionality 6.2.1 Search (Edit)).

POPD-267 - Results display

The editor page “Results” is used to

- perform the search steps preceding the diagram display
- display the set of results for the query associated with the search
- select an analysis
- display the set of results for the analysis after the query has been performed
- export the results set
- display a text representation of the query criteria
- release a search


Median-Profil-Vergleich II

eigene Recherchen - 'Median-Profil-Vergleich II' - Ergebnis

Kompartiment	Stoff	Sortier-Index	Maßeinheit	Median pro Stoff	Profil	Referenzwert	Maßeinheit Referenzwert
Boden Terrestrisch	PCB 81	202	µg/kg	5.0E-4	Boden, Bio-Freiland-Betrieb	1.6669	ng/kg
Boden Terrestrisch	PCB 167	211	µg/kg	0.00999	Boden	0.010075	
Boden Terrestrisch	PCB 105	205	µg/kg	0.02095	Boden	0.02061	
Boden Terrestrisch	PCB 123	208	µg/kg	0.00103	Boden	0.001075	
Boden Terrestrisch	PCB 167	211	µg/kg	0.00999	Boden, Bio-Freiland-Betrieb	1130.0	ng/kg
Boden Terrestrisch	PCB 77	201	µg/kg	0.004665	Boden, Bio-Freiland-Betrieb	116.4584	ng/kg
Boden Terrestrisch	PCB 77	201	µg/kg	0.004665	Boden	0.00402	
Boden Terrestrisch	PCB 81	202	µg/kg	5.0E-4	Boden	5.0E-4	
Boden Terrestrisch	PCB 114	206	µg/kg	5.2E-4	Boden, Bio-Freiland-Betrieb	16.9	ng/kg
Boden Terrestrisch	PCB 123	208	µg/kg	0.00103	Boden, Bio-Freiland-Betrieb	0.0	ng/kg
Boden Terrestrisch	PCB 189	212	µg/kg	0.00326	Boden	0.00333	
Boden Terrestrisch	PCB 126	203	µg/kg	0.00143	Boden	0.001205	
Boden Terrestrisch	PCB 157	210	µg/kg	0.00322	Boden, Bio-Freiland-Betrieb	204.0	ng/kg
Boden Terrestrisch	PCB 189	212	µg/kg	0.00326	Boden, Bio-Freiland-Betrieb	401.0	ng/kg
Boden Terrestrisch	PCB 105	205	µg/kg	0.02095	Boden, Bio-Freiland-Betrieb	512.0	ng/kg
Boden Terrestrisch	PCB 118	207	µg/kg	0.05273	Boden	0.05238	
Boden Terrestrisch	PCB 169	204	µg/kg	5.0E-4	Boden	5.0E-4	
Boden Terrestrisch	PCB 169	204	µg/kg	5.0E-4	Boden, Bio-Freiland-Betrieb	16.5839	ng/kg
Boden Terrestrisch	PCB 156	209	µg/kg	0.01795	Boden, Bio-Freiland-Betrieb	1770.0	ng/kg
Boden Terrestrisch	PCB 156	209	µg/kg	0.01795	Boden	0.01763	
Boden Terrestrisch	PCB 126	203	µg/kg	0.00143	Boden, Bio-Freiland-Betrieb	111.4989	ng/kg
Boden Terrestrisch	PCB 114	206	µg/kg	5.2E-4	Boden	5.7E-4	
Boden Terrestrisch	PCB 118	207	µg/kg	0.05273	Boden, Bio-Freiland-Betrieb	2920.0	ng/kg
Boden Terrestrisch	PCB 157	210	µg/kg	0.00322	Boden	0.00328	

Suchkriterien | Ergebnisdefinition | Ergebnis | Diagramm | Freigabe

Figure 8: Results display

Taking account of the previously defined search criteria, the results display shows the information available in the database on the results columns previously selected in the editor page “Output format” (or specified by an allocated analysis).

It also provides context menu short-cuts for displaying measuring programs and substances. Information on the measuring program can be displayed in a separate detailed screen after selecting the short-cut “Display measuring program info”, once the measuring program ID has been defined as a results column. A GSBL link is provided to a results column “CAS-No”.

The measuring program display takes the form of an overview screen for the measuring program title data that is based on the current status of the Dioxin-DB. The main purpose of this functionality is to “recruit” those users who are used to working with the existing POP-Dioxin database.

The time of day is not relevant in the data stocks used from the POP-Dioxin database. For this reason, time entries in the search application always use the format “Date” (without stating the time). Figures are always in decimal (not exponential) notation with up to four decimal places.

The heading line is displayed in **bold type**. The results currently shown in the table preview can be sorted on the basis of an individual column.

The textual representation of the search criteria for the underlying query is displayed by clicking on a button and has the following format:

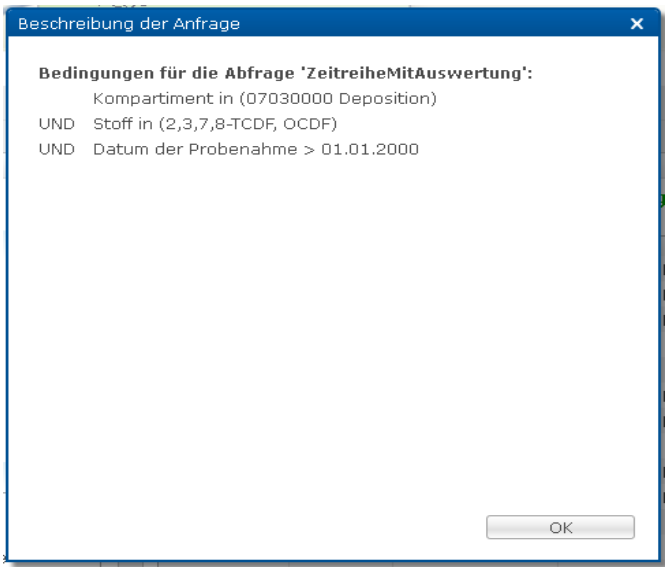

Beschreibung der Anfrage
Bedingungen für die Abfrage 'ZeitreiheMitAuswertung':
Kompartiment in (07030000 Deposition)
UND Stoff in (2,3,7,8-TCDF, OCDF)
UND Datum der Probenahme > 01.01.2000
OK

Figure 9: Query description (criteria)

The selection definition, and where appropriate also the analysis definition based on the selection, is run when the editor page “Results” is opened and displayed. The refresh button is only needed if changes in the data are expected.

POPD-266 - Allocation of an analysis definition

A dialog is provided for allocating an analysis definition to a search. This can be called by clicking on a button on the results page.

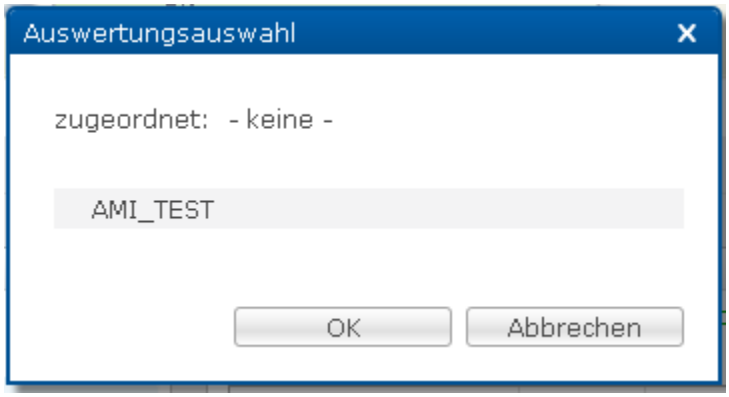


Figure 10: Analysis selection

An analysis definition to be run as part of the edited search is selected from a filtered list. The filter criterion is the interface description: the analysis definitions displayed are confined to those where the input columns match the query result provided and, if a diagram has already been allocated to the search, the output columns match the allocated presentation definition.

POPD-268 - Management dialog

A simple dialog is used to manage, i.e. to name and release searches and to deposit descriptions of the searches.
The dialog is opened by clicking a button on the results page.

The name of a search must not contain the special characters "<", ">", "[", "]" or "/", as these are needed for the textual representation of the selection definition and for controlling the ODA driver. If these characters are used, saving is not permitted. A message asks the user to alter the name accordingly.

Only a user with the role of “Editor” has the right to release a search and is offered the relevant button.

POPD-361 - Results display in diagram

As well as displaying the results as a table, the POP-Dioxin Search Application also allows the results to be presented with the aid of prepared presentation definitions.

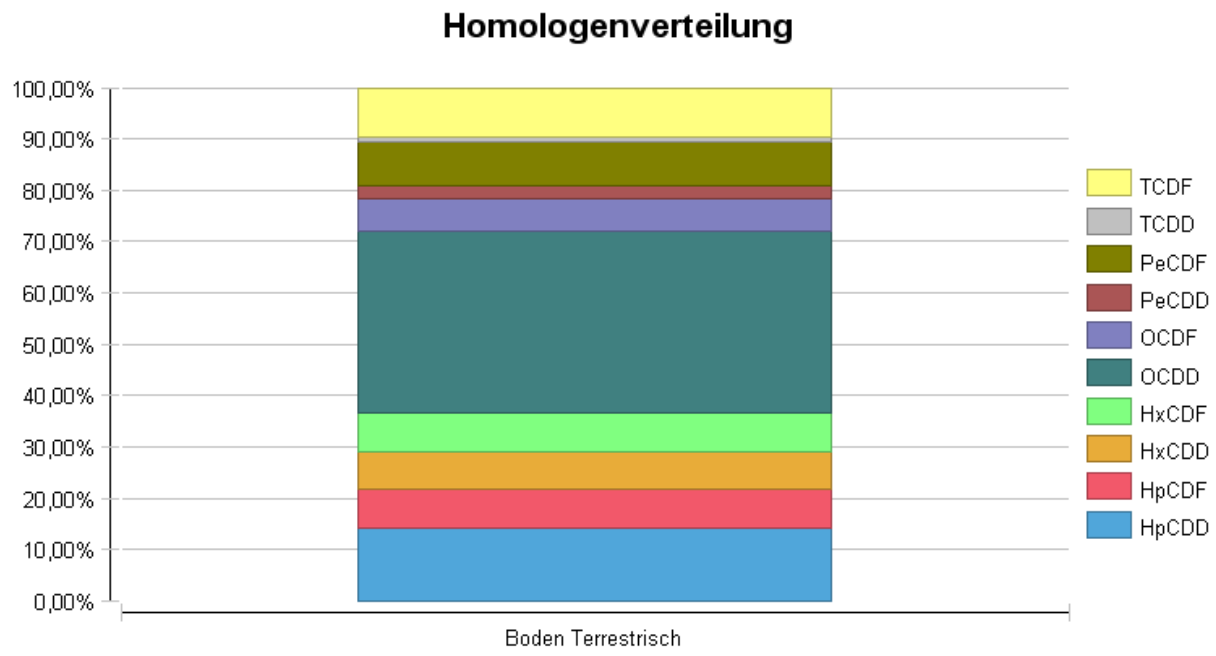


Figure 11: Results display in diagram

4.2.2 Program interfaces

POPD-427 - Search run interface

The Search module provides an interface for running searches.

The interface, implemented by means of the class “ActivityController”, has a two-stage structure:

Stage 1) Determine search results for subsequent display

Stage 2) Present the search results determined for display in a diagram, as described in the corresponding presentation definition.

4.3 Functionality

4.3.1 Functions

POPD-209 - Search management
Creating and editing searches is only possible in the private sphere (“My Searches” folder).
When a new search is created, this generates an – initially transient - data object and associates it with the current user. If the user saves the search and gives it a name, the search becomes permanent.
If the user does not save a research, closing the edit screen triggers a message to the user asking whether the search is to be saved. If the answer is “No”, the search is not saved.
Once the search is successfully saved, the user can see it in the navigation tree folder “My Searches” after refreshing the navigation pane. Here the search can be selected for further editing (action “Edit”), or to run (action “Run”) or delete it (action “Delete”).

The default view of the “Search” perspective shows only the navigation pane. After clicking on the button “New Search”, users with the role “Search Creator” are free to search, specify their own results columns and search criteria, appraise the results of the query and select a diagram for presentation. In other words it is possible to define and run a search once the “Search” perspective has been activated. The user then has the opportunity to save the newly defined search under a name of their choice.

POPD-213 - Deleting a search from the group folders
A search can only be deleted from the group folders by a user who has the role of “Editor” for the group in question.

Once a search has been marked in the group folders, the action “Delete” is available as a context menu function.

POPD-259 - Editing a search

Defining a search involves providing the necessary management information (name and description) plus exactly one query definition, not more than one analysis definition and not more than one presentation definition. Thus the minimum a search consists of is one query definition which can be run and the result exported. Optionally it is then possible to perform an analysis. Optionally, the result of the query or the result of an analysis can then be displayed with the aid of the diagram type specified in the presentation definition.

Accordingly, the user interface for defining a search has editor pages for composing a search from a query definition (comprising a description and the search criteria), an (optional) analysis definition and an (also optional) presentation definition. Editor pages are also provided for presenting the results.

The user is normally guided through the following stages:

Editing a search:
- Define search criteria for query (“Search” tab)
- Define results columns for query (“Output format” tab)
- Display result (“Results” tab)
- Allocate analysis definition (“Results” tab)
- Allocate presentation definition and display result in the diagram described by the results presentation (“Graphic display” tab)
- Release search (“Results” tab or “Graphic display” tab)

POPD-273 - Automatic addition of results columns and criteria
When a search is created, the following results columns are generated automatically:

Figure 12: Results columns

When a search is created, the following criteria for further editing are generated automatically:

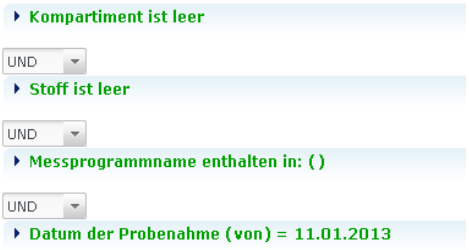


Figure 13: Criteria

In addition, a condition attached to the selection element with the key "mp7" (refers to "T_TITEL.VERTRAULICHKEIT") is automatically generated when running a search or query, depending on the role assigned to the user (see 5.1.3 Role specific conditions for controlling data visibility). This condition cannot be deleted at runtime.

Together with the saving of individual results columns (see 5.1.3 Role-specific provision of selection elements for defining results columns and criteria) this makes it possible to ensure very extensive protection of confidential information.

POPD-212 - Releasing a search

A search has to be released to make it available for running by other users, namely the members of the group for which the search is released.

A search is released for a group from the editor page “Results”. When performing the action “Release” it is always necessary to specify the target group. Only those groups to which the current user is assigned with the role of “Editor” are offered for releasing.

When releasing the search, it is also necessary to include the group for which the corresponding query definition was released. Since the query definition is created together with the search, the query definition is released together with the search for the same group.

When a user’s private search is released, it is first saved, then copied and the copy is allocated to the group specified for release. Following releasing and subsequent refreshing of the navigation pane, the released search is available to the user in the navigation pane folder for the specified group.

The released search can no longer be edited in the target group’s folder. Any changes to the released search that are made in the folder “My Searches” remain local, i.e. they are not synchronized with the copies in the group folders.
If a search copied to the group folders needs to be updated, it first has to be deleted in the group folder. Then it can be released again. There must not be two searches with identical names for a group.

POPD-260 - Running a search
Searches that have been defined and saved can be run any desired number of times. When running a search, search criteria defined in the query definition by the expert user may be offered for the current user to enter freely selectable values. This is done in two stages corresponding to the relevant tabs:

Performing a search:
- Define search criteria
- Display result

When performing a search, all the individual activities described by the query, analysis and presentation definitions allocated to the search are run in sequence.

POPD-293 - Exporting results
The result of a search before the presentation definition is displayed can be exported (see also 4.2.1 Results display).

This is subject to the following conditions:

- The time of day is not relevant in the data stocks used from the POP-Dioxin database. For this reason, time entries in the search application always use the format “Date” (without stating the time).
- The result is exported to exactly one table / worksheet.
- When exporting, a legend is generated on a separate worksheet. The content entered in the legend is the textual representation of the selection definition, the name of the search, the user name and the creation time.

POPD-274 - Changing results columns and criteria when performing a query or search
The procedure for protecting confidential information must not be undermined by deleting results columns or criteria in “Run” mode. Neither must anything be done to destabilize the interaction of query, analysis and presentation. The following restrictions therefore apply:

- Deleting criteria in “Run” mode is only permitted if the results column is marked as “editable”. (Reason: protection of confidential information)
- Deleting results columns in “Run” mode is not permitted. (Reason: functional efficiency of assigned presentations/analyses)

4.4 Data model

POPD-413 - Data model for search

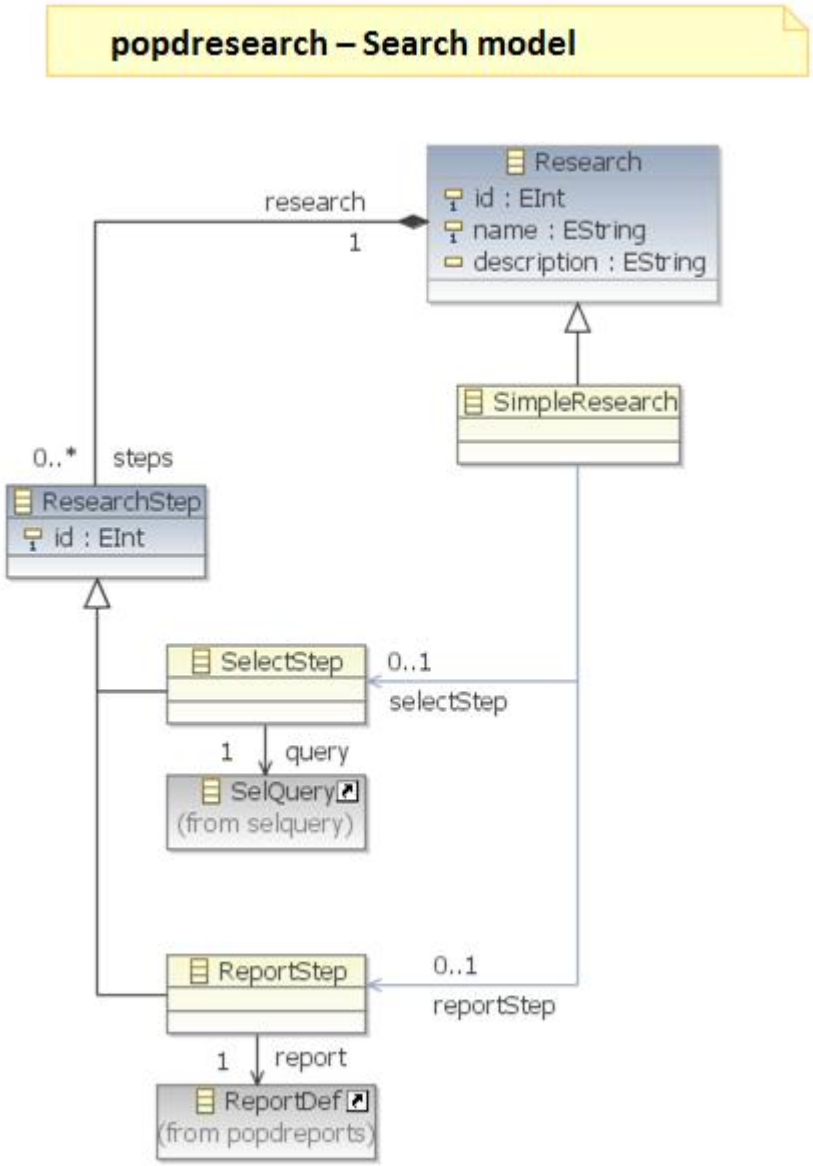


Figure 14: Data model "Search"

POPD-414 - Data model for data transfer interface

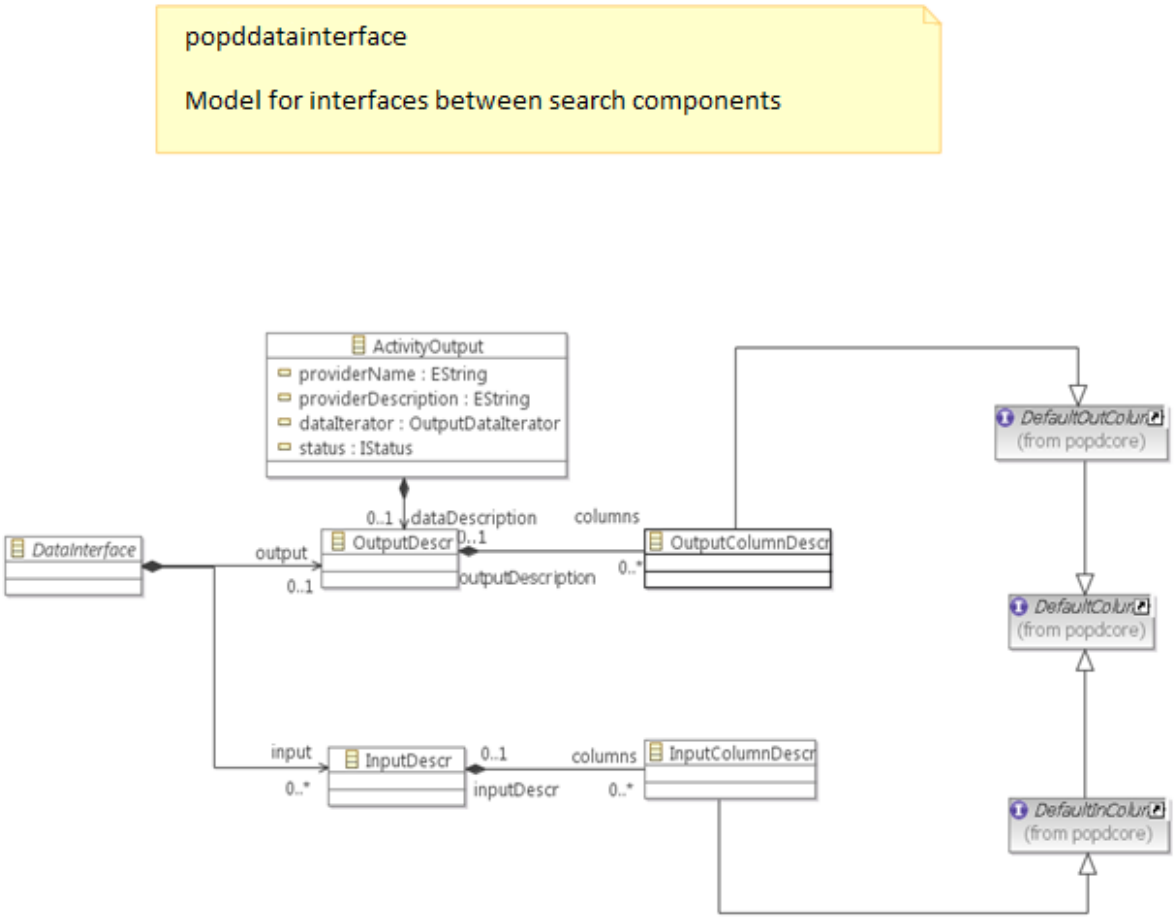


Figure 15: Data model "Value transfer"

4.5 Interfaces used

POPD-306 - Transfer of values between the modules

The result of a query definition is transferred – as an interim result – to the "Analysis" module for running the analysis definition. The result of running the analysis definition – again as an interim result – is transferred to the presentation module for display. It is also possible to transfer a query result – as an interim result – directly to the presentation module. The interim results are transferred in tabular form, and the structure and form of the transferred values are described by metadata.

Interim results are "cached" within the search application. This involves handling large sets of results. For this purpose a maximum application-wide figure (30,000) is laid down for the number of elements (results rows) in a set of results. Initially all results rows are determined up to the index corresponding to the specified maximum value. If this figure is exceeded, an error message appears, asking the user to further restrict the set of results. This procedure is designed to prevent the

processing of excessive quantities of results from exceeding the system resources of the application server or web server and thereby endangering the operation of the system as a whole.

POPD-310 - User interface for maintaining metadata
A standardized user interface for maintaining metadata is provided for the modules “Analysis” and “Presentation”.

POPD-305 - Interfaces for running a search
A search is run by performing, one after the other, , the individual activities defined for the search in the sequence: query, analysis (if appropriate), presentation (if appropriate). This is done using the program interfaces of the modules “Selection”, “Analysis” and “Presentation”.
Execution of the individual steps in the search is centrally controlled via a uniform interface.

POPD-304 - Interfaces for interface testing
The specified metadata are used to check that the information provided is compatible with the information expected.
Interface checking is performed with the aid of a standardized data structure (see 4.4 Data model value transfer interface).

5 Rights module

5.1 Description of the module

User guidance in the “POP-Dioxin Search Application” is based on a simple but powerful authorization (rights) strategy.

1) The functionality of the POP-Dioxin Search Application can be linked to one or more roles. Only users who are members of the specified roles are allowed to use the relevant functionality.

2) Access to information is controlled by group membership. The application’s configuration data can be assigned to groups.

It is also possible to combine control by role and group membership: If use of a function is restricted by group membership and by a role, the current user not only has to be a member of the group that is allowed to use the function, but must also be assigned the required role for this group.

An authorization check is performed to decide whether a specific function can be offered to the current user. A user’s right to use a particular function is checked by determining the roles assigned to the user and comparing them with the roles allowed to use the function. If access to a function, e.g. displaying specific selection tree elements in the “Selection” module, is controlled by a group-role combination, the user’s membership of the relevant role-group tuple is verified before access to the function is permitted.

Users are assigned to groups and roles by means of the user interfaces of the Rights module.

5.1.1 Groups

POPD-378 - User groups
The user groups for the POP-Dioxin Search Application are divided up on the basis of expert subject topics. The groups used for organizing access to the application data (searches and query definition) are as follows:

- **Air**
- **Water**
- **Soil**
- **Food**
- **Measurement and research programs**
- **Standard**

POPD-231 - User guidance control by means of group membership
Allocation to groups is used largely for configuration of the navigation pane, i.e. the display of group folders for searches and queries.
Users are shown only the group folders for the groups to which they are assigned in user management.
Below the group folders a list of all searches released for this group that the user can perform is displayed without any further substructure.

5.1.2 Roles

POPD-377 - Roles for user-specific control of the functions offered by the search application
The roles required for the search application are:

- **User administrator:** permits user configuration
- **Application administrator:** permits the provision of analyses and diagrams
- **Search creator:** permits definition of own (free) searches
- **Editor:** permits the provision of searches for other users in a user group
- **Search subscriber:** permits execution of searches belonging to a user group
- **Special user**: permits execution of predefined searches, confidentiality level 1 [confidential]
- **Expert user:** permits execution of predefined searches, confidentiality level 2 [for internal use]
- **User:** permits execution of predefined searches, confidentiality level 3 [for third parties] and changes to own password

The roles assigned to the current user are shown in the status bar.

5.1.3 Data visibility

Data visibility in the “POP-Dioxin Search Application” is controlled by two complementary mechanisms.

POPD-261 - Role-specific conditions for controlling data visibility
Data views are implemented via a role-specific, automatically completed and non-deletable condition for the confidentiality stage (1 [confidential], 2 [for internal use], 3 [for third parties]) of the measuring program (Table "T_TITEL"). When a query is submitted, this condition is dynamically added to the query depending on the role assigned to the user:

- If the user has the role “User” or none of the roles listed here, the condition "T_TITEL.VERTRAULICHKEIT = 3" is added.
- If the user has the role “Expert user”, the condition "T_TITEL.VERTRAULICHKEIT = 2" is added.
- If the user has the role “Special user”, the condition "T_TITEL.VERTRAULICHKEIT = 1" is added.

The data in the table T_TITEL, like all measurement data associated with this table (database table T_ANALYSEERGEBNIS) from the selection result, are filtered according to this condition.

If the value of the column "VERTRAULICHKEITSSTUFE" for an entry in the table "T_TITEL" is "NULL", this is treated as the same as the value "3". This means that this entry and the associated data are visible to all users with the roles “Special user”, “Expert user” and “User”.

No data visibility restrictions are made in the BIRT Designer environment, which means that all information necessary for creating meaningful presentations is available when drawing up the presentation definitions.

POPD-262 - Role-specific provision of selection elements for defining results columns and criteria
Selection tree elements affected by data visibility restrictions are linked in the metadata with roles and, where appropriate, groups. The syntax is:
- "RESTRICTED: " + <Rolename> + "::" + <Groupname>
or
- "RESTRICTED: " + <Rolename>
This allows the use of a selection element to be restricted either
- for users who have been assigned the specified combination of role and group
or
- for users who only need to be assigned the specified role.

The current user’s right to use the relevant selection tree element is checked when defining the queries.

5.1.4 Configuration

POPD-379 - Interaction between groups and roles
In the POP-Dioxin Search Application, the following functions are controlled depending on assignment to roles and groups:

- Data access: see 5.1.3 Role-specific conditions for controlling data visibility
- Availability of selection tree elements: see 5.1.3 Role-specific provision of selection elements for defining results columns and criteria
- Release functionality: is controlled by the role “Editor” for the assigned group
- Availability of searches in a user group: is controlled by the role “Search Subscriber” for the assigned group
- Free search: is permitted for users with the role “Search Creator”
- User administration: is permitted for users with the role “User Administrator”
- Availability of analyses and diagrams: is permitted for users with the role “Application Administrator”

A new user is assigned the roles “User” and “Search Creator”.
The user “Guest” is not assigned any role.

The roles **User Administrator, Application Administrator** and **Search Creator** are sufficiently configured without being assigned to any group. In the search application the rights to perform administration tasks and to define free searches are determined without reference to any groups assigned.

The roles **Special User** (confidentiality level 1 [confidential]), **Expert User** (confidentiality level 2 [for internal use]) and **User** (confidentiality level 3 [for third parties]) control access to data (see 5.1.3 Role-specific conditions for controlling data visibility).
If a user is assigned one of these roles, assignment to a group is only necessary if access is to be permitted to selection tree entries with group-specific access restrictions (see 5.1.3 Role-specific provision of selection elements for defining results columns and criteria).
At present the selection tree sheets “Soil Use” (restriction to role “Special User” and group “Soil”), “Industrial Facilities” (restriction to role “Special User”) and “Easting (location)” and “Northing (location)” (restriction to role “Expert user”) are filtered.
What this means for user configuration is that, for example, access to the information “Industrial Facility” is possible for all users with the role “Special User”. By contrast, a user who is to be assigned the right to view the information “Soil Use”, has to be explicitly assigned the tuple {role “Special User”, group “Soil”} in the user administration.

The role of **Editor** should always be assigned to a user as a tuple with a specific group. If a user is an editor for a group, he is allowed to provide searches for precisely this group. Only an editor has the right to delete searches for his group.

The role of **Search Subscriber** is the counterpart to the role of **Editor.** The role of **Search Subscriber** should also always be assigned to a user as a tuple with a specific group. If users are search subscribers for a group, the search overview offers them all searches made available to the members of the group by the group editors.

The availability of the following functionalities is controlled by showing or hiding the relevant menu items/buttons:

- Administration: only active for users with the role “User”. In particular, this means that only users with the role “User” can change their password.
- User administration: only active for users with the role “User Administrator”
- Provision of analyses and diagram definitions: only active for users with the role “Application Administrator”
- Creating new searches, creating and saving own searches, adding results columns and new criteria to existing searches: only active for users with the role “Search Creator”. If this role is not assigned, the selection list for “My Searches” in particular is not available. Copying searches from a group is also only possible for users with the role “Search Creator”.
- “Release” button: only available for users with the role “Editor”. The groups available to an editor when releasing a search are determined in the user administration by specifying a group for the role of “Editor”. It is possible to be an editor for more than one group.

5.2 Interfaces

5.2.1 Masks

POPD-219 - User rights administration screen
The user rights administration screen makes it possible to manage user details.
It also allows creation and deletion of assignments between users, groups and roles. A user with the role “User Administrator” has the right to assign users to groups and roles, and to authorize access to the search application.

5.2.2 Program interfaces

POPD-228 - Authorization check
Three test methods – "hasRole(<Rolename>)" "hasGroup(<Groupname>)" and "hasRoleForGroup(<Rolename>,<Groupname>)" – are made available for the authorization check via the application framework (class "UserContext").
The methods provide information on whether the current user is assigned a specific role, a specific group or a specific combination of role and group.
All authorization checks within the application context are performed using these methods.
POPD-229 - Determining group membership for a user
For group folders to be displayed in the navigation tree, it is necessary to determine the group(s) to which the user is assigned. The application context (class "UserContext") therefore provides the method "getGroups", which makes it possible to find out all groups of which the current user is a member.

5.3 Functionality

5.3.1 Functions

POPD-222 - Creating, editing and deleting users
Selecting the menu item “Administration/Users” results in the navigation pane displaying a list of all users registered in the system. It is then possible to create users in the navigation pane (action “New”) or edit them (action “Edit” after selecting a user in the list).

The administration section of the search application provides an editor for editing user information. The structure of the editor is simple, with a simple entry box for each attribute. Saving the details of an application user is linked to a plausibility check which ensures that all important information on the user is recorded in the system. Assignment to groups and roles is done in the same editor.

One important action in the context of user administration is authorizing a user account described by the administration interface for active use of the system. The user cannot log into the system until the authorization has been activated (remove “Blocked” flag).

User accounts marked in the list in the navigation pane can also be deleted from the system completely (action “Delete”). However, this is only possible if the user is no longer assigned any searches or queries.

POPD-226 - Defining and deleting user-role-group assignments
A user can be assigned roles and groups in the user administration editor.
The user interface for assigning roles and groups to a user is structured as a simple table with columns for group and role. Groups, roles and users are assigned to each other by adding a new row to the table. An assignment is deleted by selecting a row in the table and deleting it (action “Delete”).

POPD-341 - Rights information on configuration objects
Configuration objects used to control the application can be implemented as a “ProtectedObject”. This permits assignment to groups or users which can be checked at runtime, to determine processing rights. The search definitions and the query definition are implemented as “ProtectedObject”.

5.3.2 User administration

The user administration as a functional unit makes use of the functions described in Section 5.3.1 above. The following administration workflow is supported:

- Creating a user
- Assigning roles

The available roles and their effects on the application are described in Section “5.1.2 Roles”. A meaningful minimum configuration for a newly created user should contain the role assignments **“User”** and **“Search Subscriber”** for the group **“Standard”**. Other roles (e.g **“Search Creator”** or **“Editor”**) can be added at any time to assign additional rights to a user.

6 Selection module

6.1 Description of the module

The "Selection" module is used to define database queries from the point of view of the expert domain. A query definition created using the POP-Dioxin Search Application can be saved in the system. The query definition saved in the system contains all information necessary for submitting an SQL query to the underlying DB system and suitably preparing the set of results. The user interface of the module is designed to ensure that it is intuitive and easy to learn for the expert user.

Abstraction from the technical data model

To make it as simple as possible for expert users to find the data they need, and to make it unnecessary for them to acquire and maintain a sound technical knowledge of the technical data model, the user interface provided for defining database queries and deciding the results set structure and filter criteria for a database query is free from technical terminology.
The main advantages of this approach are:

- Users do not need a profound knowledge of the data model
- Queries can be created from the point of view of the expert user

The appearance of the user interface for defining the results structure and filter criteria is configured. This configuration involves a large degree of abstraction from the technical data model, which is one of the crucial features of the search application (see 6.3.1 Configuring the Selection module).

After configuration, the tree view shown in the user interface for defining the results structure and filter criteria for a query might look like this, for example:

On the basis of this "**selection tree**", very few steps are needed to create a query:

1. Selecting and editing the filter criteria
The first step is to select the filter criteria from the selection tree for further editing, and then carry out the necessary editing. Various relational operators can be used depending on the data type.

2. Determining the scope of the information

Then the information needed for displaying the results is selected (see 6.2.1 Search / Filter Definition ff.).

3. Results display
The results set can then be determined on the basis of the setting made above (see 6.2.1 Selection / Results Display).

6.2 Interfaces

The "Selection" module provides

- external user interfaces for making a query definition available (definition of search and filter criteria, results structure and aggregation rules) and
- program interfaces for performing a saved query definition within the Search module.

6.2.1 Screens

The user interfaces of the Selection module are used to define queries. Initially the management and execution of definitions only takes place within the search definition and execution process. However, the application architecture already makes provision for a future extension, which is therefore included in this description of the solution.

POPD-162 - Search / Filter definition
The “Search” editor page is used to define filter criteria. Here filter criteria can be added, edited and deleted.

The criteria shown in the user interface are separated by the string " - AND - " or " - OR - ". The string is implemented as a “link”. Clicking on the string changes the operator from "AND" to "OR", or vice versa. Such changes are only permitted in Edit mode.

A block of criteria linked by "OR" is always indented.
The relational operator is shown before each element of the list of criteria, except for the first element.

From the presentation of the results (see 4.2.1 Results Display) it is possible to display a textual representation of the criteria, the structure of which is based on the structure described here.

The editor page “Search” can be opened in both “Run” and “Edit” modes. Only the “Edit” mode gives the user the full range of facilities for defining filter criteria. To simplify user guidance, the “Run” mode only permits editing of predefined filter criteria.
POPD-420 - Search (Edit)
In the “Search” editor page it is possible to describe filter criteria in a query by selecting the individual criteria and establishing a relationship with a reference value.

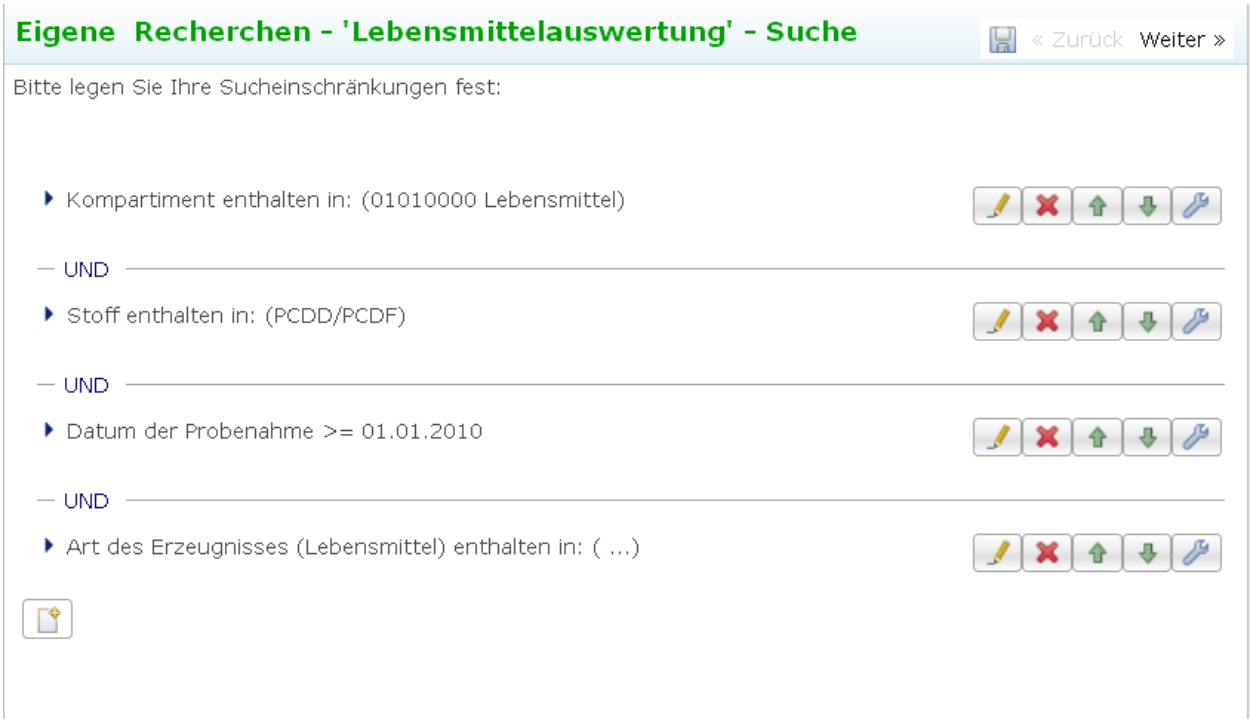
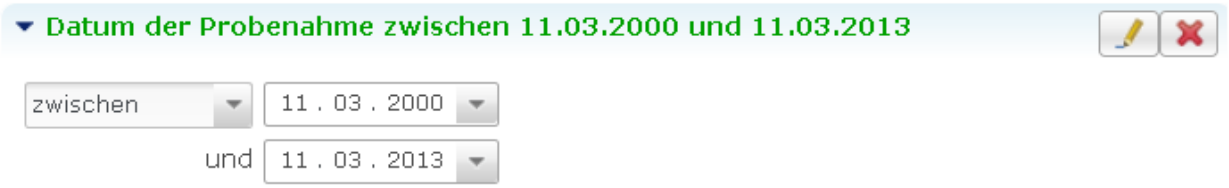

Eigene Recherchen - 'Lebensmittelauswertung' - Suche
« Zurück Weiter »
Bitte legen Sie Ihre Sucheinschränkungen fest:
Kompartiment enthalten in: (01010000 Lebensmittel)
UND
Stoff enthalten in: (PCDD/PCDF)
UND
Datum der Probenahme >= 01.01.2010
UND
Art des Erzeugnisses (Lebensmittel) enthalten in: (...)

Figure 16: Search

A separate “section” (e.g. “compartment in...” in the above screenshot) is displayed for each criterion of the query.
The sections can be expanded to specify relational operators and reference values.
If a criterion for a query definition is protected, it is no longer possible to alter relational operators or reference values for the criterion at runtime.

POPD-264 - Search (Run)
In Run mode, all filter criteria prepared in Edit mode are displayed. Once a section has been expanded, the criteria can be edited, but only if the criterion was declared “editable” when the search or query was defined.



If the criterion is protected, it is no longer possible to alter the reference values or relational operators. In that case a textual description of the criterion is displayed when the section is expanded.

POPD-344 - Catalogs

The catalogs that form the basis for the list and tree views of the criterion editors draw their data from the same data source as is used for the results data. Hierarchical data models (parent/child relationship) are needed for the tree view. The catalogs are configured like the selection trees.

View of catalogs:

A catalog node is marked in grey if at least one reference value is selected in the branch below the node.
A node is marked in grey if a node above the leaf is selected as a reference value.

A node that is marked in grey can be selected by clicking on it. The nodes above and below are colored according to the rules mentioned.

POPD-265 - Results definition

In the editor page “Output format” the results structure for a query can be described by selecting the individual columns of the results table. Results columns can be added and deleted. They can also be marked as a sort criterion or linked to an aggregation function.

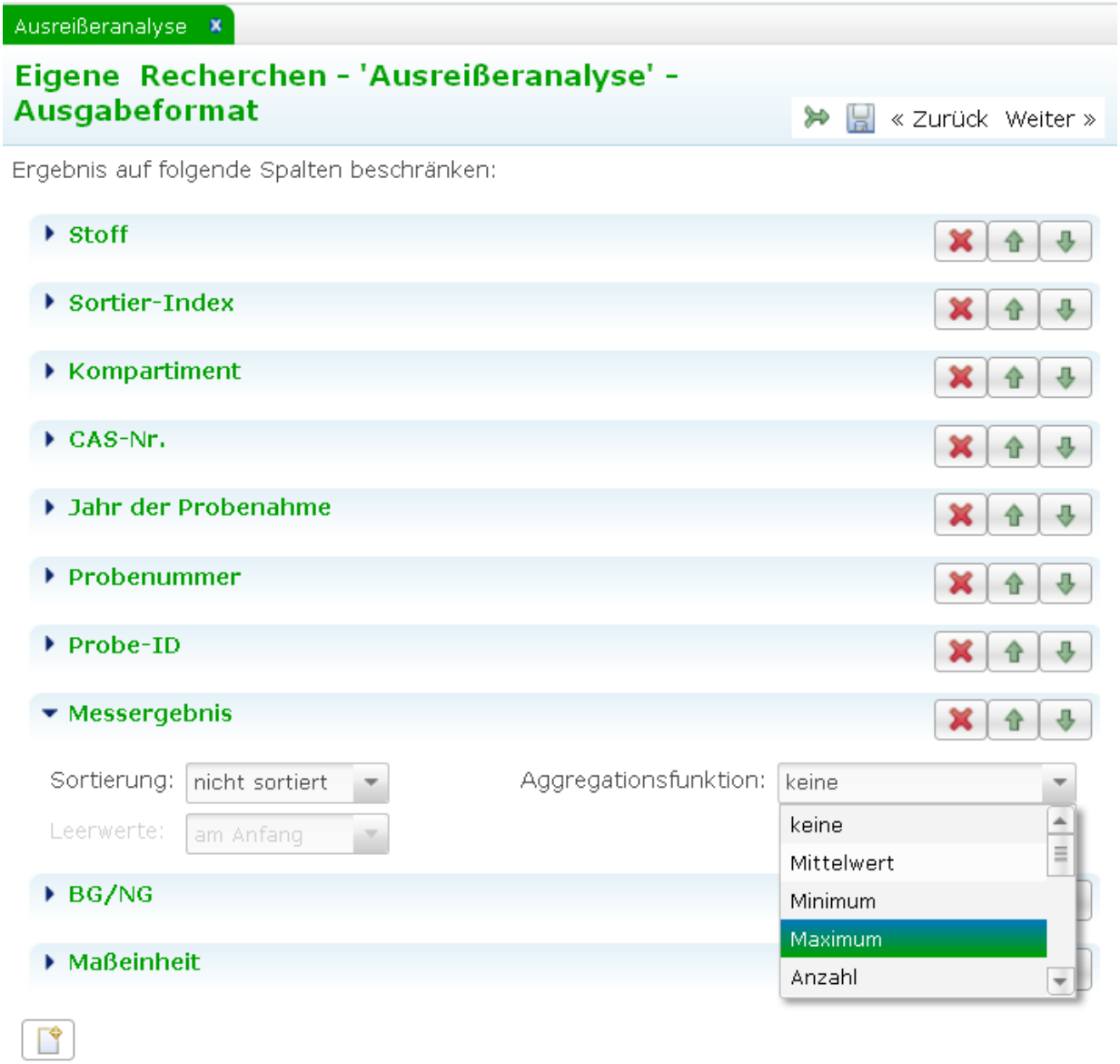


Figure 17: Aggregation

To aggregate a results column (e.g. measurement) in the editor page “Output Format”, it is possible to select an aggregation function after selecting or expanding the section in order to edit the results column to be aggregated. The aggregation functions provided are the 1st, 10th, 25th, 50th (median), 75th, 90th, and 99th percentiles, max, min and number.
The result is a results column that contains the defined aggregation result when the query is run.
All other results columns selected in the editor for results definition purposes are used as a grouping criterion, unless they are themselves subject to aggregation.

A results column may be selected more than once and may in each case be linked with different aggregation functions. For example, a results column with a different aggregation function that

delivers the number of values included in the (first) aggregation result, may also be declared by the user a second time.

POPD-163 - Selection / Results Display
The selection results are presented with the aid of the editor page “Results” (see 4.2.1 Results Display) from the Search module.

6.2.2 Program interfaces

POPD-429 - Interface for running queries
The “Selection” module has a “SelectionActivityController” interface which the search component uses to run the query definition assigned to a search saved in the system.

6.3 Functionality

The entire functionality of the Selection module is concerned with defining and running database queries by the expert user, the aim being to make it easy and convenient to retrieve meaningful technical information from the data stored in the Federal and Länder Dioxin Database.

6.3.1 Functions

POPD-230 - Selection tree
The features for defining a query can be selected from the selection tree. The contents of the selection tree are controlled by means of a configuration file.
Using the selection tree, individual features or all features grouped under a node can be added to the results column list or the criteria catalog. Multiple selections are also possible.

POPD-221 - Configuring the Selection module
The first step in configuring the Selection module is to identify those sections of the overall data model which are relevant to the search and make them available for defining selection trees for display in the user interface. This in itself is a very important abstraction step. Then the features made available are given technically meaningful names, grouped and – where appropriate – assigned additional metadata. The metadata are used at runtime to display the selection tree provided in the user interface for creating queries.

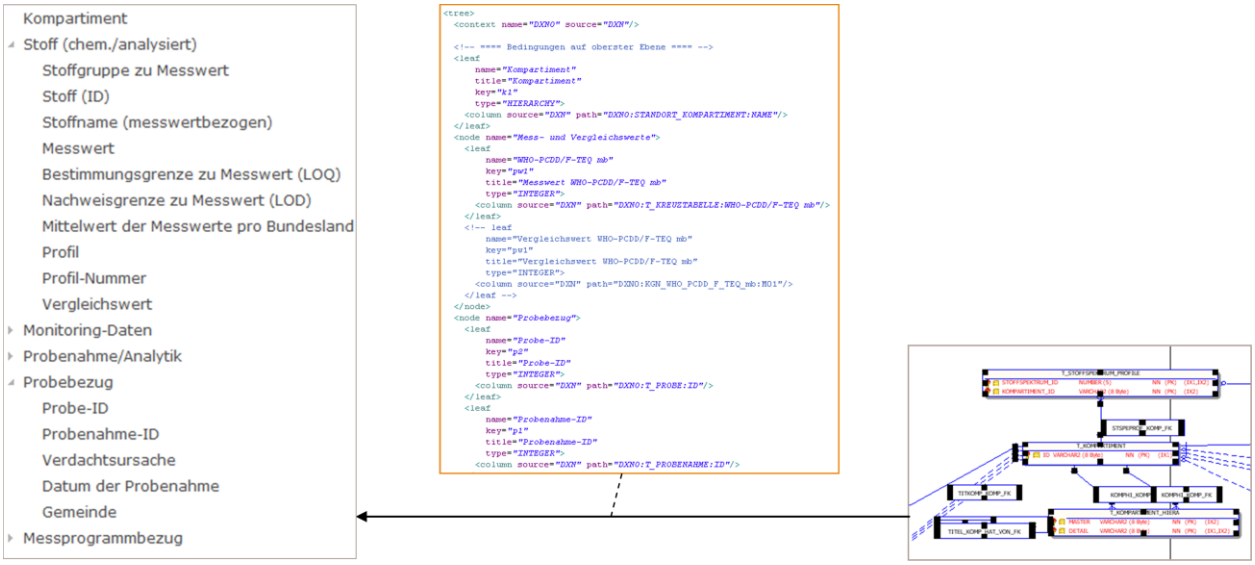


Figure 18: “Selection tree” concept

The configuration of the Selection module can even be extended and modified while the system is running. This ensures a large measure of flexibility and extensibility for the operation of the POP-Dioxin Search Application as a whole.

POPD-366 - Condition editors

Data type specific editors allow the user of the search application to maintain conditions. Two classes of editors are distinguished:

a) Editors for reference values (in list or tree form), which are used to assign reference values from the database via catalogs to the criteria selected by means of the selection tree.

b) Editors for simple reference values/literals. This may be a date value, for example.

POPD-165 - Filter variables

One special feature of the POP-Dioxin Search Application is the facility reserved for expert users for defining variable filter criteria. For any desired filter criterion it is possible to specify that its reference values may be changed by the user performing the search. Typical examples of this include the selection of a sample ID, a period or a location reference.

POPD-338 - Catalogs

It is possible to define catalogs for criteria selection. These definitions are also saved in the database and managed with the aid of an SQL script "UPDATE_CATALOGS.sql", which is maintained by Condat.

POPD-329 - Conditions analysis

Conditions are defined depending on their type. There are:

a) different condition editors and relational operators for different data types, and

b) different representations in the database for the data type “Boolean” (Yes/No).

The search application supports the implementation of Boolean values as numeric entries in the database.
This implementation observes the following conventions:

- the value NULL means FALSE
- the value 0 (numeric null) also means FALSE
- all values except NULL and 0 mean TRUE

In SQL the conditions are as follows:

- query column COL for FALSE: (COL is null or COL = 0)
- query column COL for TRUE: COL != 0
  (in this comparison, SQL implicitly adds the condition "COL is not null"!)

In the event of further database representations for Boolean values, a more far-reaching solution would be a new condition type, e.g. BOOLEAN_Y_N, which can be used in seltree.xml and is treated differently in the QueryToSelectionTranslator than the existing type BOOLEAN.

The relational operators EQ, NEQ, IN and NOT_IN are implemented for Boolean conditions.
IN with an empty value results in the condition 1 = 0
IN with the value set (TRUE, FALSE) results in no condition at all.

POPD-335 - Undefined conditions
To ensure that a query always yields a result, incompletely defined conditions are not permitted.
It is also important to ensure that the relative lack of restrictions on result definitions does not lead to very large results sets and hence performance problems.
For this reason the default condition is set to "is empty" or "is NULL", since this can be expected to yield a relatively small set of results.
If a criterion is not completely defined, this should where possible be visually highlighted in the criterion editor.

POPD-232 - Linking conditions
Criteria may be linked by "AND" or "OR".
"OR" always takes priority over "AND".
No other linking of filter criteria is provided.

POPD-299 - Running a query
When running a query, duplicate results sets are filtered to hide redundant information from the user.
For all results columns in the set of results, first all corresponding entities (within the meaning of ER modelling) are selected. This is done by taking the PK column(s) of all tables whose results columns were specified in the results definition and adding them to the columns selected in the SQL query submitted. In this way any duplicates are filtered out of the resulting results set. This eliminates any technical duplicates that may, for example, result from the SQL-JOIN construct. By contrast, any duplicates of sectoral relevance, e.g. measurements that happen to be identical, are delivered to the user in the results set. This is important for subsequent analysis of the results data with the Analysis module, and also for the aggregation function within the Selection module.

POPD-331 - Comparison of metadata when performing queries
The creation of SQL statements within the selection requires unique identification of the metadata on the database scheme or data model.
Important metadata on the data model includes in particular:

- Database and scheme
- Database tables
- Columns in database tables

Because there are differences between the concepts of Hibernate (recommends overwriting the "equals" methods in the Java classes) and EMF/Teneo (advises against this) in the context of object identification, the methods businessEquals() and businessHashCode() are used within the POP-Dioxin Search Application for content-related identification of SelContext, SelTable, SelColumn.
In addition, the following aids are provided for development:

- Wrapper classes for `SelContext`, `SelTable`, `SelColumn`, to use the above-mentioned methods for `equals()` and `hashCode()`. The wrapper classes give warnings of the type "SelColumn.businessEquals() is inconsistent with equals(): {} <--> {}", if objects from different sessions are indeed mixed.
- `java.util.Set` implementations for `SelTable` and `SelColumn`, which make internal use of the wrapper classes.
- `java.util.Map` implementation for `SelTable`, which makes internal use of the wrapper class for `SelTable`.
- Use of these `Set` and `Map` implementations in the `select.core` package for correct treatment of the same `SelTable` and `SelColumn` objects loaded in different Hibernate sessions (different Java objects referencing the same instances in the database).

POPD-332 - Treatment of data types
Data types are output in standardized form in the POPD Search Application. As well as numeric data types and character strings, which are used by the POP-Dioxin Search Application in their canonical representation specified by the database, this applies to date formats and Boolean values:

- Date: dd.MM.yyyy
- Timestamp: dd.MM.yyyy HH:mm
- Boolean: 1/0

6.4 Data model

The most important data model in the selection component is the model for describing the expert data model abstracted via the selection tree. The structure of the metadata offered via the selection tree is described in the "select.core" model.

POPD-159 - Model select.core

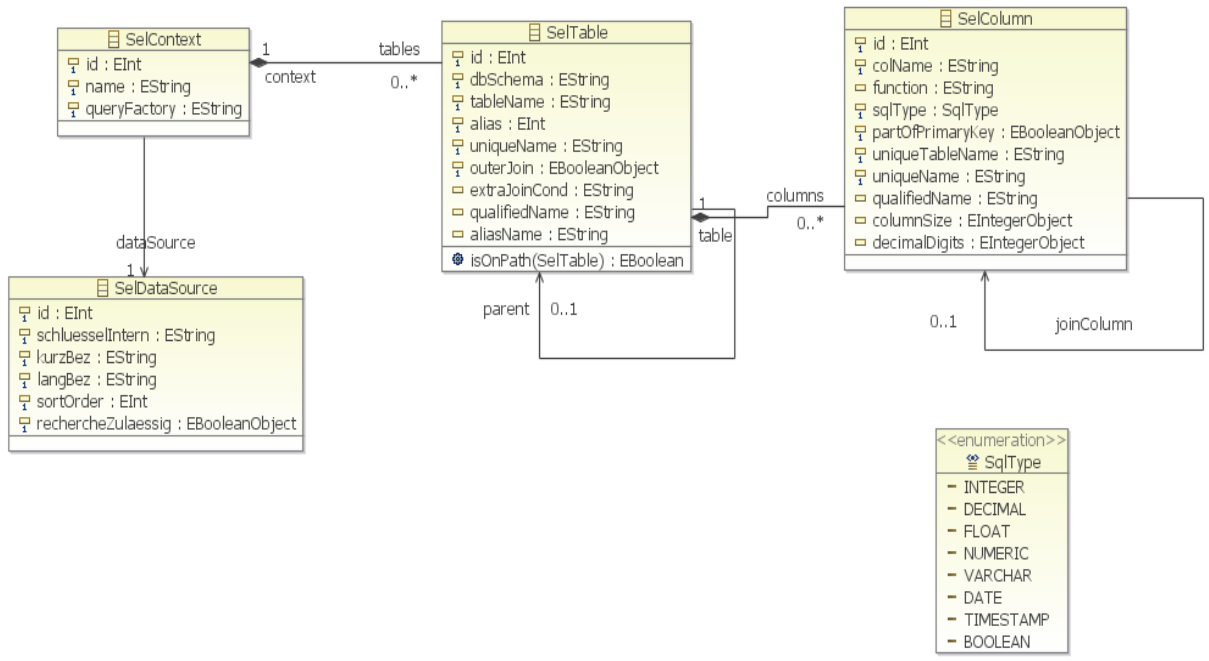


Figure 19: Data model "Selection"

7 Analysis module

7.1 Description of the module

The "Analysis" module is used to run R-scripts that have previously been made available in a separate runtime environment with tools by the manufacturer "Revolution Analytics".

Before running them it is necessary to save metadata in the search application about the structure of the input expected by the R-script and the structure of the results returned. In this solution concept the metadata is known as the "Analysis definition".

When a search – consisting of query definition, analysis definition and presentation definition – is performed, the query result is determined. Then an R-script identified in the analysis definition is started in the "Revolution Analytics" runtime environment using the transferred query results set, and the analysis result is returned.

All R-scripts used for searches are created and provided by the UBA. An exported selection result in Excel format can serve as the basis for creating a new R-script.

The entry and result are transferred in tabular form – in each case as exactly one table.

The R-scripts must ensure error treatment for the parameter transfer – by calling "R.Event.On()" at least for incomplete or incorrect input data. Condat provides the UBA with exemplary advice on creating an R-script suitable for the search application and creating the corresponding analysis definition.

7.2 External interfaces

The “Analysis” module provides

- the external user interface “R-Connector” for providing an analysis definition (name, description, R-script-name, metadata on expected input and result) and
- program interfaces for running a saved analysis definition within the Search module.

7.2.1 Screens

POPD-245 - Screen for providing an analysis definition
The screen for providing an analysis definition largely corresponds to the screen for providing a presentation definition. In both cases the search application is supplied with metadata for running external applications (R-script or BIRT report).

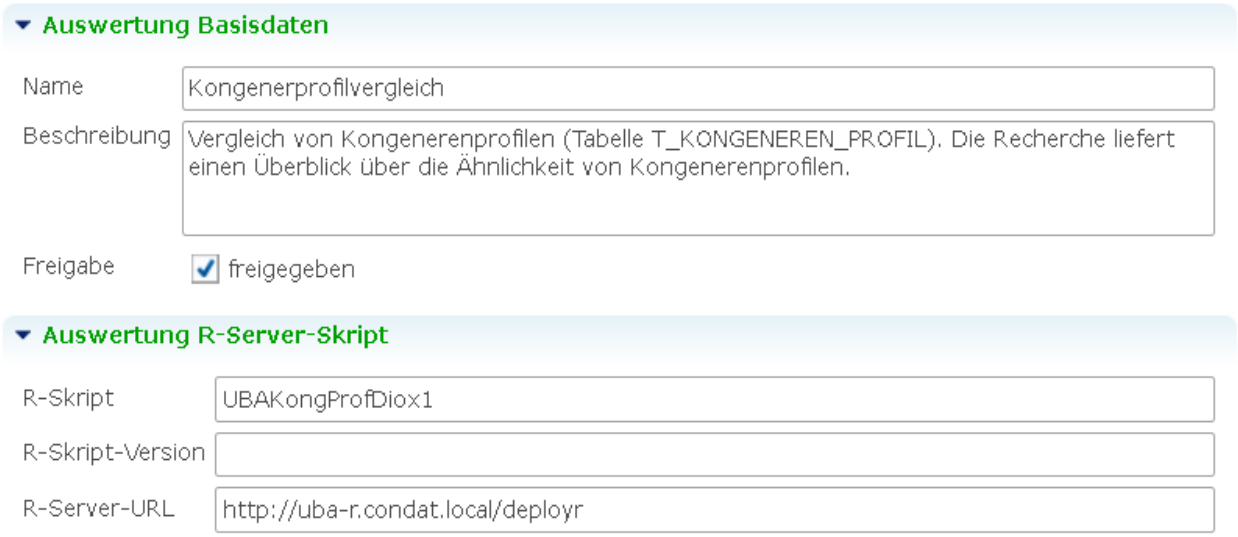


Figure 20: Providing an analysis definition

For an analysis definition, facilities are provided for specifying input and results columns. This allows the script creator to provide information about the structure of the returned results, thereby enabling the search application to validate the values transferred to the presentation module.

7.2.2 Program interfaces

POPD-247 - Interface for running an analysis
The “Analysis” module has an “AnalysisActivityController” interface which the search component uses to run the analysis definition assigned to a search saved in the system.

7.3 Functionality

The functionality of the analysis module consists of the functionality for providing new R-scripts and the functionality for running these R-scripts when performing a search.

7.3.1 Functions

POPD-199 - Creating an analysis definition in the Administration section
An “analysis definition” consists of

- Name of analysis
- Description
- Full URL (incl. protocol "http://") of the R-script directory in the “Revolution” environment, consisting of Server Name, Port Number and directory path (in a standard installation: "deployr")
- Details of input columns
- Details of results columns

When an analysis definition is created, this information is obtained from the expert and then saved in the runtime environment of the POP-Dioxin Search Application.
If the analysis definition is assigned to a search, the following steps are performed by the POP-Dioxin Search Application when running the search:

- Check whether the results columns of the query definition to which the search is assigned correspond to the expected input of the analysis definition
- Run the query associated with the search
- Extract the results set for the query
- Transform the results set into an R-specific representation
- Using the URL of the R-script, call the saved R-script and transfer the query results set as an R-object
- Determine the results set of the R-script and make it available for presentation (here too a check is made to see whether the results columns of the analysis definition correspond to the expected input of the presentation definition)

POPD-200 - Editing an analysis definition in the Administration section
An analysis definition can be edited until it is released.

By the time the analysis definition is released, the expert must ensure that the input columns and the results columns specified in the R-script are saved correctly and completely in the analysis definition, in order to ensure trouble-free functioning of the analysis module within the search application.

POPD-289 - Tree for selecting results columns in an analysis definition
A tree similar to the selection tree is provided for selecting results columns for an analysis. Configuration of the possible results elements takes place in consultation with the UBA and is performed by Condat. The tree contains all selection tree results columns configured for the

selection module, which means the relevant values can simply be “passed through”. However, it also contains analysis-specific results columns, so these additional results of the analysis are available for the presentation as well (BIRT Report definition).

POPD-207 - Releasing an analysis definition
Unlike the procedure for the modules “Selection” and “Search”, an analysis definition is released simply by setting the flag “Released”.
In other words there is no group-specific release, neither are analysis definitions copied on release.

POPD-290 - Running an analysis definition
The following steps are performed when running an analysis definition (precondition: an R-script was made available in the “Revolution” environment and the “POP-Dioxin Search Application” was supplied with the corresponding metadata):

1) Determine query result
2) Create an R-object from the query result
3) Make the created R-object (query result) available in the R-runtime environment and start the R-script for analysis
4) Determine the result of the R-script, a newly created R-object
5) Transform the result into a POPD-compliant Java representation

POPD-201 - Deleting an analysis definition in the Administration section
An analysis definition may only be deleted if it has not yet been released.

7.4 Data model

POPD-248 - Data model for analysis definition
The data model for an analysis definition comprises the following information:

- Released
- Name of analysis
- Description
- URL of the R-directory in the “Revolution” environment
- Details of input columns
- Details of results columns

7.5 Interfaces used

POPD-256 - Interface with REvoDeployR/Revolution Analytics
The libraries provided by “Revolution Analytics” are called via their interfaces and used to run an analysis definition, transfer the query results and take over the analysis results.

8 Presentation module

8.1 Description of the module

The “Presentation” module is used to display query and analysis results determined by the search application. For this purpose the “Presentation” module makes use of the open-source software “BIRT”.

BIRT supports the generation and presentation of reports on the basis of two components: A Report Designer tool based on Eclipse, and a runtime component integrated in the search application.

If a new presentation is to be made known to the search application, it is first necessary to create a new “Report Definition” with the Report Designer tool.

Then metadata on the structure of the input expected by the presentation must be saved in the search application. The complete metadata needed for the results presentation is referred to here as “Presentation definition”. A presentation definition is provided with the aid of the “BIRT Report Connector” (see 8.3.1 Creating a presentation definition in the Administration section.)

When running a search, consisting of query definition, analysis definition and presentation definition, the query result is determined and, if appropriate – after subsequent analysis of the query result – the analysis result. The report definition stored in the metadata on the search is used in the BIRT runtime environment to display the transferred data as a diagram.

All presentation definitions used for searches are created and provided by the UBA. Condat provides support with the integration of the BIRT Report Designer functionality and gives the UBA exemplary advice on creating a report definition.

8.2 Interfaces

The “Presentation” module provides

- the user interface “BIRT Report Connector” for providing a presentation definition (name, description, report design name, meta-information on expected input) and
- program interfaces for performing a saved presentation definition within the Search module.

8.2.1 Screens

POPD-245 - Screen for providing a presentation definition

The editor for providing a presentation definition largely corresponds to the screen for providing an analysis definition. In both cases the search application is supplied with metadata for running external applications (R-script or BIRT report).

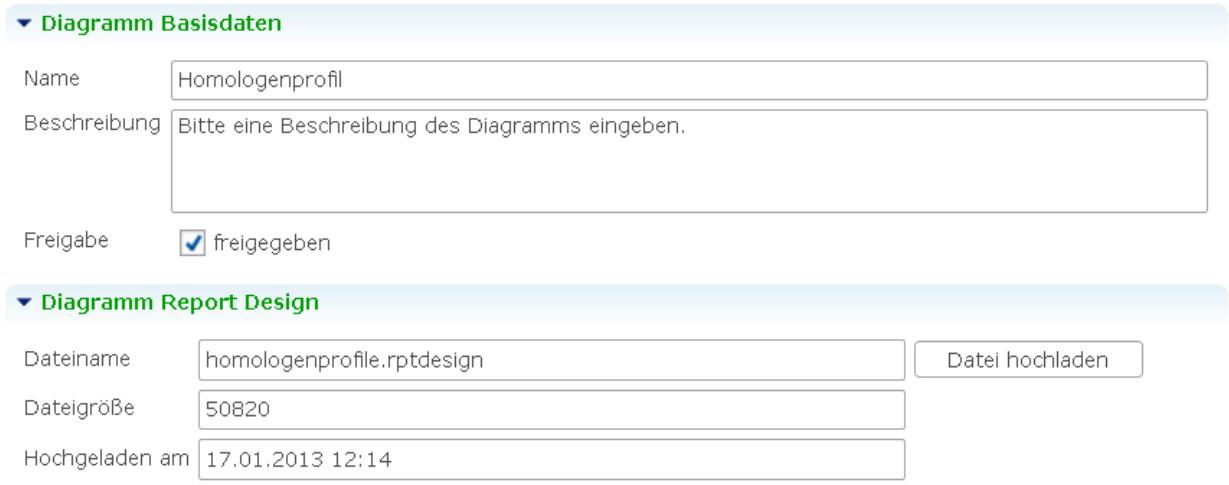


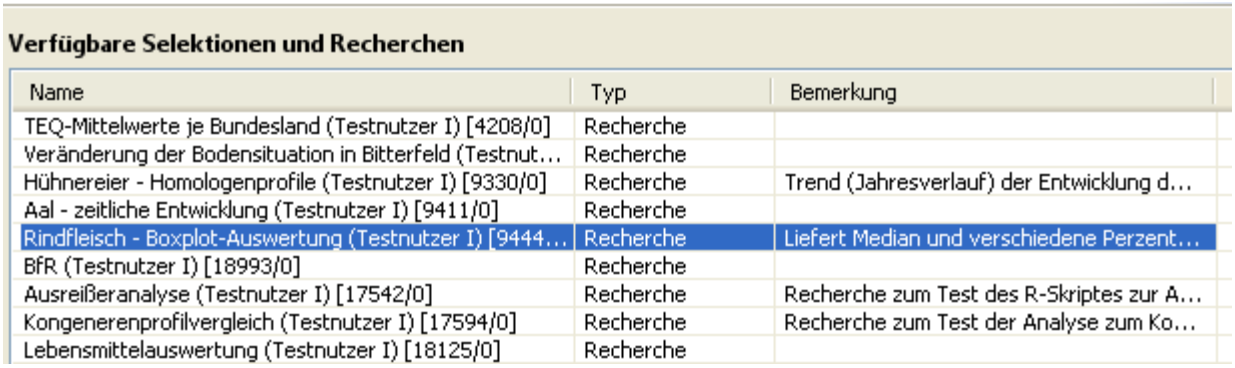
Figure 21: Providing a presentation definition

In addition to the metadata on the Report Design file, the expected input columns are specified. It is possible to add and delete input columns. When defining a search and running a search, the assigned input columns are used to check whether the presentation definition is compatible with the query or analysis to be run before it.

Unlike the analysis definition, no definition of results columns is needed for the presentation definition.

POPD-423 - Report Design definition screen

One important element in the search application is the extension of the BIRT Designer, which makes it possible to use existing searches as early as the report drafting stage.

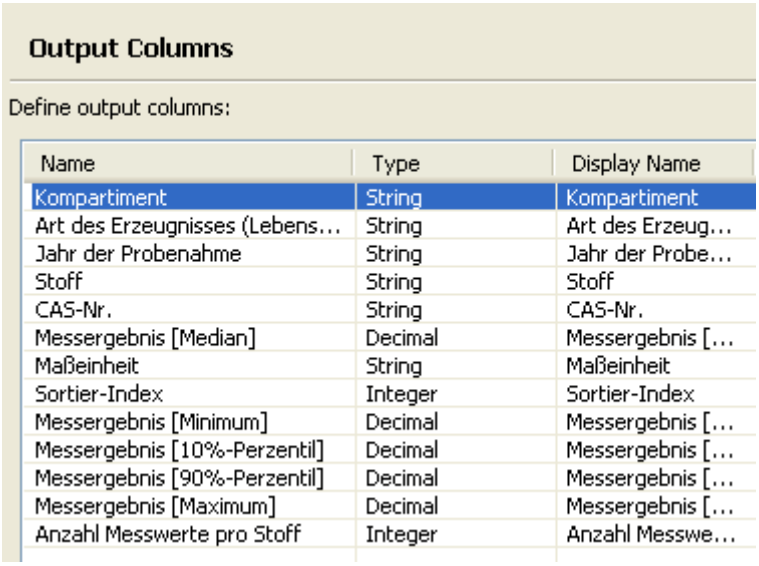


Verfügbare Selektionen und Recherchen

Name	Typ	Bemerkung
TEQ-Mittelwerte je Bundesland (Testnutzer I) [4208/0]	Recherche	
Veränderung der Bodensituation in Bitterfeld (Testnut…	Recherche	
Hühnereier - Homologenprofile (Testnutzer I) [9330/0]	Recherche	Trend (Jahresverlauf) der Entwicklung d…
Aal - zeitliche Entwicklung (Testnutzer I) [9411/0]	Recherche	
Rindfleisch - Boxplot-Auswertung (Testnutzer I) [9444…	Recherche	Liefert Median und verschiedene Perzent…
BfR (Testnutzer I) [18993/0]	Recherche	
Ausreißeranalyse (Testnutzer I) [17542/0]	Recherche	Recherche zum Test des R-Skriptes zur A…
Kongenerenprofilvergleich (Testnutzer I) [17594/0]	Recherche	Recherche zum Test der Analyse zum Ko…
Lebensmittelauswertung (Testnutzer I) [18125/0]	Recherche	

Figure 22: Selecting a search (BIRT)

The BIRT Designer uses the same descriptors as in the search application for the results columns.



Output Columns

Define output columns:

Name	Type	Display Name
Kompartiment	String	Kompartiment
Art des Erzeugnisses (Lebens…	String	Art des Erzeug…
Jahr der Probenahme	String	Jahr der Probe…
Stoff	String	Stoff
CAS-Nr.	String	CAS-Nr.
Messergebnis [Median]	Decimal	Messergebnis […
Maßeinheit	String	Maßeinheit
Sortier-Index	Integer	Sortier-Index
Messergebnis [Minimum]	Decimal	Messergebnis […
Messergebnis [10%-Perzentil]	Decimal	Messergebnis […
Messergebnis [90%-Perzentil]	Decimal	Messergebnis […
Messergebnis [Maximum]	Decimal	Messergebnis […
Anzahl Messwerte pro Stoff	Integer	Anzahl Messwe…

Figure 23: Available information (BIRT)

This means that provision of the report design does not involve any break in the application concept either. This fulfils the requirement that users must be provided with access to the information to be presented that is independent of the technical database technology and based on their own expert terminology.

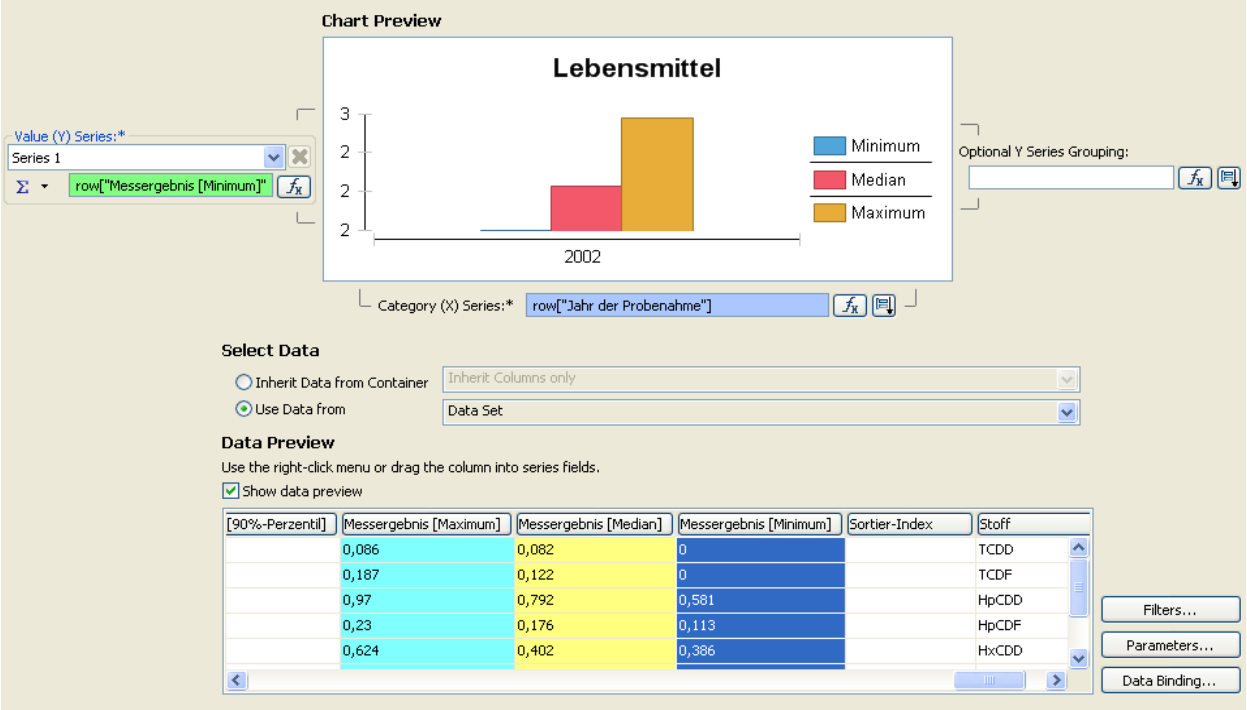


Figure 24: Diagram definition (BIRT)

8.2.2 Reports

POPD-252 - Creating reports for presenting results sets

The BIRT Report Designer can be used to define reports based on searches previously defined under the “POPD Search Application”. All private (i.e. not yet released) searches available in the system are offered, so that an expert can construct adequate presentations on this basis. The reports created can be registered with the POPD Search Application, enabling them to be used for presenting query and analysis results as part of a search.

8.2.3 Program interfaces

POPD-254 - Interface for running a presentation

The “Presentation” module has a “ReportController” interface which the search component uses to run the presentation definition assigned to a search saved in the system in order to display a results set as a diagram.

8.3 Functionality

The functionality of the presentation module consists of the functionality for providing new BIRT report designs and the functionality for generating reports on the basis of the report design when running a search.

8.3.1 Functions

POPD-269 - ODA driver
For integration in the BIRT Report Designer there is an “ODA driver”. When defining new reports this makes it possible to access searches previously defined with the search application from the BIRT Report Designer.

POPD-199 - Creating a presentation definition in the Administration section
A “presentation definition” consists of

- Name of presentation
- Description
- Name of BIRT Report Design file
- Details of input columns

When a presentation definition is created, this information is saved by the expert in the runtime environment of the POP-Dioxin Search Application.
Any presentation definitions with input columns that do not match the results columns of the query or – if appropriate – the analysis are filtered out by the selection dialogs for assigning a presentation definition.

POPD-195 - Editing a presentation definition in the Administration section
A presentation definition can be edited until it is released.

When a presentation definition is edited, it is in particular uploaded to the POPD environment.

The following messages may appear on upload:

- Unknown report data source: The input columns must be explicitly specified
- A results column in the search used to define the BIRT report has been deleted: Check and if necessary update the report definition.

On release at latest, the expert must ensure that the input columns are specified in the presentation definition.

POPD-207 - Releasing a presentation definition
Unlike the procedure for the modules “Selection” and “Search”, a presentation definition is released simply by setting the flag “Released”. In other words there is no group-specific release, neither are presentation definitions copied on release.
The presentation definition cannot be assigned to a search until it has been released, i.e. after the flag “Released” has been set to “true”.
The “Released” flag for a presentation definition should only be reset from “true” to “false” if the presentation definition has not yet been used in a search.

POPD-283 - Using a presentation definition
The presentation definition is used when performing a search. For this purpose the results of the previous individual search steps are determined. The result is transferred to the presentation

module, which in turn uses the POPD-ODA driver (see 8.3.1 ODA driver), to display the results.

The following activities are performed when running a presentation definition:

- Run the query (and, if appropriate, the analysis) associated with the search
- Extract the results set
- Check whether the results columns of the query definition or analysis definition correspond to the input expected by the presentation definition.
- Call the saved BIRT report design
- Display the diagram generated on the basis of the results set and the report design

POPD-196 - Deleting a presentation definition in the Administration section
A presentation definition may only be deleted if it has not yet been released. It may only be deleted if it has not yet been assigned to a search.

8.4 Data model

POPD-255 - Data model for presentation definition
The data model for a presentation definition comprises the following information:

- Released
- Name of presentation
- Description
- Name of BIRT Report Design file
- Details of input columns

8.5 Interfaces used

POPD-257 - Interface with BIRT runtime environment
BIRT libraries are used to generate diagrams for displaying query and analysis results. Generation of the diagrams is based on the BIRT Report Design file specified in the presentation definition and is controlled by the interfaces of the BIRT runtime environment.

9 Analyses with R / congener profile comparison

9.1 Analyses with R

The POPD Search Application uses the software "R". A previously compiled data query, together with the selected statistical options, can be transferred to R, which uses standard routines to prepare and analyze it. The results are passed to the HTML screen for downloading and/or display.

The Revolution Analytics Management Console (Fig. 1) is used to upload R-scripts to the Deploy-R environment, give them a name and release them for a specific user group. The web-based application enables any number of source texts (not *.r files!) to be uploaded to the R server.

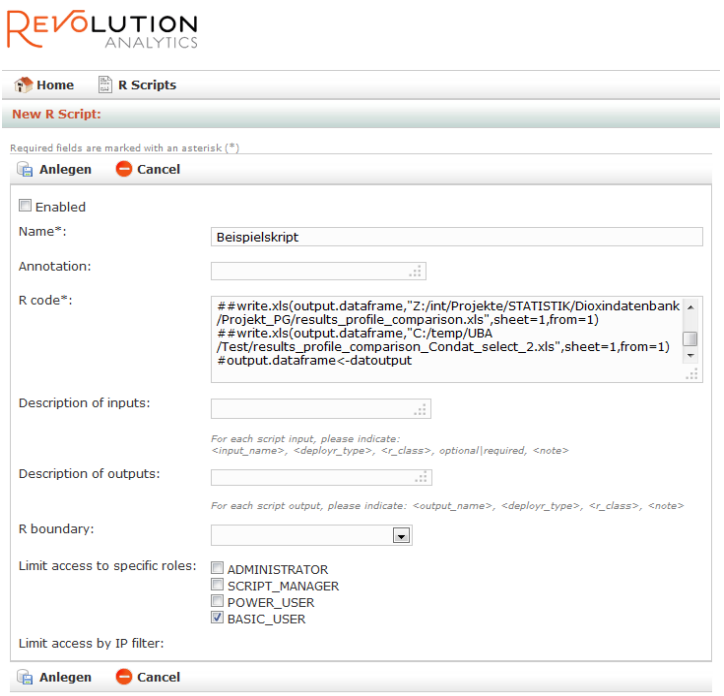


Figure 25: Revolution Analytics Management Console

The analyses previously defined in the code are thus available on the R server and can be released for search results on the "Administration" tab of the POPD Search Application (Fig. 2). The crucial factor is that the set of input columns (the output format for the results) and the output are specified in accordance with the definitions of the R-script. The application provides user guidance tailored to these settings.

Figure 26: Administration interface "Analyses"

It is essential to specify the exact character string for the name of the script and the URL of the R server, which corresponds to the web address of the Management Console (within the DMZ).

An R-analysis does not have to be used exclusively for results sets corresponding to the requirements of the input definitions. For example, if "Compartment", "Substance", "Measurement", "Detection limit" and "Measurement unit" are defined as input for an analysis, the mechanism can also be used for searches that show "Sampling Year", "CAS-No." or similar as results. If one of the input elements is missing, however, it is not possible to activate the analysis.

Once the search criteria and output formats have been defined, R-analyses can be selected in the "Results" tab (Fig. 3).

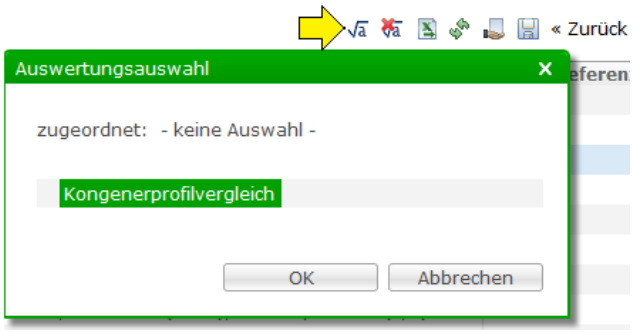


Figure 27: Selecting an analysis (access to R-scripts)

Confirming the dialog with "OK" automatically updates the results set, and the result of the calculations is then output. Click on the icon to return to the search result (without R-analysis).

9.2 Congener profile comparison

Chemical compounds with the same structure form a “congener pattern”, indicating sources of a particular kind with similar contamination. The database makes it possible to compare distribution patterns with the archived sample data. This permits rapid and reliable identification of contamination sources, an important step towards improving the safety of food and animal feeds, for example.

To this end a first methodological approach has been implemented with the aid of mathematical scaling and distance determination. Every comparison of the contaminated sample with a potential contamination source results in a corresponding scaling factor (k_i) and distance ($dist_i$). It must be remembered that a congener pattern is primarily characterized by the mutual relationships of the individual congeners, and not by their absolute measured values. This leads to the conclusion that a congener profile is scalable. The closer together two (scaled) profiles are, the greater their similarity, so all that is needed now is to calculate the distances of the scaled individual concentrations from the concentrations of the contaminated profile.

In a further development stage the data model was adapted to cater for the planned deposition of contamination and source patterns, the congener profiles. A deliberate decision was taken to implement separate storage of congener profiles and data from measurement programs (Fig. 4). With the aid of foreign key references it is possible to establish a relationship between profiles and measurement programs. This takes account of special studies involving pollutant transfer.

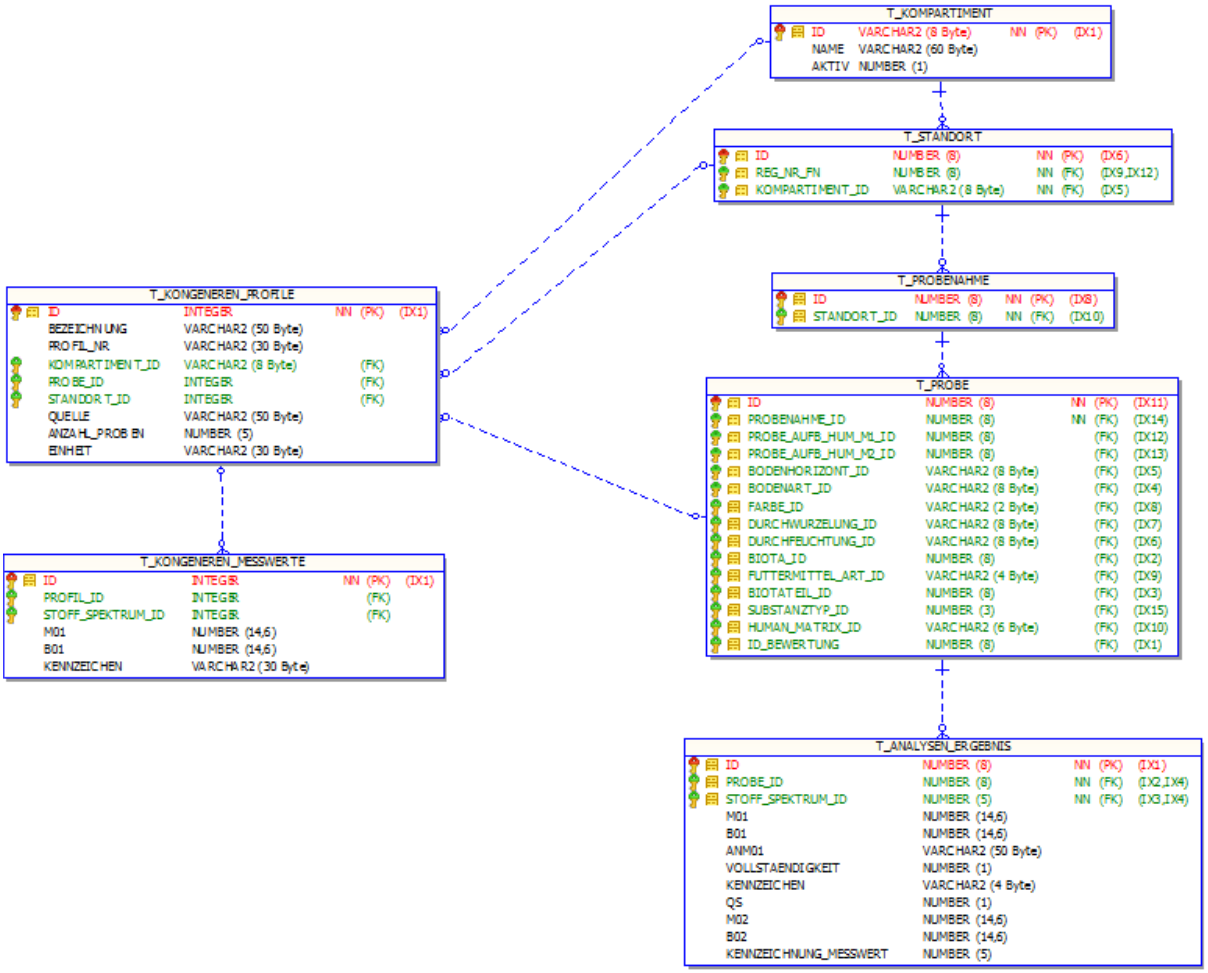

T_KOMPARTIMENT
ID VARCHAR2 (8 Byte) NN (PK) (IX1)
NAME VARCHAR2 (60 Byte)
AKTIV NUMBER (1)
T_STANDORT
ID NUMBER (8) NN (PK) (IX6)
RBG_NR_FN NUMBER (8) NN (FK) (IX9,IX12)
KOMPARTIMENT_ID VARCHAR2 (8 Byte) NN (FK) (IX5)
T_PROBENAHME
ID NUMBER (8) NN (PK) (IX8)
STANDORT_ID NUMBER (8) NN (FK) (IX10)
T_KONGENEREN_PROFILE
ID INTEGER NN (PK) (IX1)
BEZEICHNUNG VARCHAR2 (50 Byte)
PROFIL_NR VARCHAR2 (30 Byte)
KOMPARTIMENT_ID VARCHAR2 (8 Byte) (FK)
PROBE_ID INTEGER (FK)
STANDORT_ID INTEGER (FK)
QUELLE VARCHAR2 (50 Byte)
ANZAHL_PROBEN NUMBER (5)
EINHEIT VARCHAR2 (30 Byte)
T_PROBE
ID NUMBER (8) NN (PK) (IX11)
PROBENAHME_ID NUMBER (8) NN (FK) (IX14)
PROBE_AUFB_HUM_M1_ID NUMBER (8) (FK) (IX12)
PROBE_AUFB_HUM_M2_ID NUMBER (8) (FK) (IX13)
BODENHORIZONT_ID VARCHAR2 (8 Byte) (FK) (IX5)
BODENART_ID VARCHAR2 (8 Byte) (FK) (IX4)
FARBE_ID VARCHAR2 (2 Byte) (FK) (IX8)
DURCHWURZELUNG_ID VARCHAR2 (8 Byte) (FK) (IX7)
DURCHFEUCHTUNG_ID VARCHAR2 (8 Byte) (FK) (IX6)
BIOTA_ID NUMBER (8) (FK) (IX2)
FUTTERMITTEL_ART_ID VARCHAR2 (4 Byte) (FK) (IX9)
BIOTATEIL_ID NUMBER (8) (FK) (IX3)
SUBSTANZTYP_ID NUMBER (3) (FK) (IX15)
HUMAN_MATRIX_ID VARCHAR2 (6 Byte) (FK) (IX10)
ID_BEWERTUNG NUMBER (8) (FK) (IX1)
T_KONGENEREN_MESSWERTE
ID INTEGER NN (PK) (IX1)
PROFIL_ID INTEGER (FK)
STOFF_SPEKTRUM_ID INTEGER (FK)
M01 NUMBER (14,6)
B01 NUMBER (14,6)
KENNZEICHEN VARCHAR2 (30 Byte)
T_ANALYSEN_ERGEBNIS
ID NUMBER (8) NN (PK) (IX1)
PROBE_ID NUMBER (8) NN (FK) (IX2,IX4)
STOFF_SPEKTRUM_ID NUMBER (5) NN (FK) (IX3,IX4)
M01 NUMBER (14,6)
B01 NUMBER (14,6)
ANM01 VARCHAR2 (50 Byte)
VOLLSTAENDIGKEIT NUMBER (1)
KENNZEICHEN VARCHAR2 (4 Byte)
QS NUMBER (1)
M02 NUMBER (14,6)
B02 NUMBER (14,6)
KENNZEICHNUNG_MESSWERT NUMBER (5)

Figure 28: Data structures for congener profiles with references

The descriptive information in the profiles is deposited in the following format:

ColumnName	ColID	PK	Null	DataType	Histogram
ANZAHL_PROBEN	8		Y	NUMBER (5)	None
BEZEICHNUNG	2		Y	VARCHAR2 (50 Byte)	Frequency
DATUM_PROBENAHME	10		Y	DATE	None
EINHEIT	9		Y	VARCHAR2 (30 Byte)	None
ID	1	1	N	INTEGER	None
KOMPARTIMENT_ID	4		Y	VARCHAR2 (8 Byte)	Frequency
PROBE_ID	5		Y	INTEGER	None
PROFIL_NR	3		Y	VARCHAR2 (30 Byte)	None
QUELLE	7		Y	VARCHAR2 (50 Byte)	None
REF	11		Y	CHAR (2 Byte)	None
STANDORT_ID	6		Y	INTEGER	None

The structure of the measured values in the profiles is based on that of the analytical results of the measurement programs. This ensures that the standardized value combination “Sample-Substance-Measurement-Detection limit” is preserved.

On the basis of the data in the extended Oracle tables, contaminated congener profiles can be determined within the POPD Search Application (Fig. 5) and possible similar source patterns can be selected for comparison (Fig. 6).

Figure 29: Selection of a contaminated profile

[REF] Basilikum, gerebelt OLS-BU-0141.2011 01010000
[REF] Basilikum Kraut 100% pur, gerebelt 11010218 01010000
[REF] Boden, Bio-Freiland-Betrieb 284465 04010000
[REF] Branntkalk OS 1201543 10000000
[REF] Einzelfutter 10126626 02000000
[REF] Gehalte in Depositionsproben in Bayern - null
[REF] Hofsammelmilch, landwirtschaftl. Betrieb 2012/03009/7 01010100
[REF] Hofsammelmilch, landwirtschaftl. Betrieb 2012/03010/4 01010100
[REF] Hofsammelmilch, landwirtschaftl. Betrieb 2012/03011/2 01010100
[REF] Kanechlor, technisch (Japan) KC-1000 null

Figure 30: : Selection of several contaminated profiles

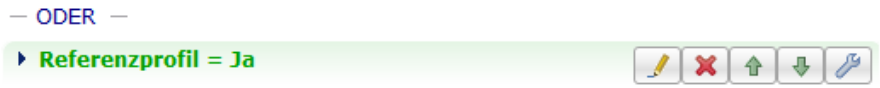


Figure 31: Selection of all potential source profiles

In the second step the output format (Fig. 8) can be scaled using the methods in the R-script and taken over into the distance determination.

Figure 32: Required transfer format for sample analyses

For each contaminated profile, the script looks for the source profile with the greatest statistical similarity. This is identified in the results column “Most similar profile”. The value shown there corresponds to a profile ID (Fig. 9) and indicates the most similar sample in a specific reference sample.

Profil ID	Quelle	Referenzwert	Ref	Profilname	Sortier-Index	Referenz BG/NG	Profilnummer	Stoff	ähnlichstes_Profil
66	DioxinDB	14,5		Mediane der PCDD/F-Gehalte i	114	0	-	2,3,4,6,7,8-HxCDF	5
66	DioxinDB	303		Mediane der PCDD/F-Gehalte i	115	0	-	1,2,3,4,6,7,8-HpCDF	5
66	DioxinDB	89		Mediane der PCDD/F-Gehalte i	116	0	-	1,2,3,4,7,8,9-HpCDF	5
66	DioxinDB	1.118		Mediane der PCDD/F-Gehalte i	117	0	-	OCDF	5
69	LUFA-Prüfbericht LV4-RU-0008-2012	0		Styropor	101	0,2	OS 1201544	2,3,7,8-TCDD	4
69	LUFA-Prüfbericht LV4-RU-0008-2012	0		Styropor	102	0,2	OS 1201544	1,2,3,7,8-PeCDD	4
69	LUFA-Prüfbericht LV4-RU-0008-2012	0		Styropor	103	0,2	OS 1201544	1,2,3,4,7,8-HxCDD	4
69	LUFA-Prüfbericht LV4-RU-0008-2012	0		Styropor	104	0,25	OS 1201544	1,2,3,6,7,8-HxCDD	4
69	LUFA-Prüfbericht LV4-RU-0008-2012	0		Styropor	105	0,2	OS 1201544	1,2,3,7,8,9-HxCDD	4
69	LUFA-Prüfbericht LV4-RU-0008-2012	1,24		Styropor	106	0	OS 1201544	1,2,3,4,6,7,8-HpCDD	4
69	LUFA-Prüfbericht LV4-RU-0008-2012	10,1		Styropor	107	0	OS 1201544	OCDD	4
69	LUFA-Prüfbericht LV4-RU-0008-2012	0		Styropor	108	0,2	OS 1201544	2,3,7,8-TCDF	4
69	LUFA-Prüfbericht LV4-RU-0008-2012	0		Styropor	109	0,2	OS 1201544	1,2,3,7,8-PeCDF	4
69	LUFA-Prüfbericht LV4-RU-0008-2012	0		Styropor	110	0,2	OS 1201544	2,3,4,7,8-PeCDF	4
69	LUFA-Prüfbericht LV4-RU-0008-2012	0		Styropor	111	0,2	OS 1201544	1,2,3,4,7,8-HxCDF	4
69	LUFA-Prüfbericht LV4-RU-0008-2012	0		Styropor	112	0,2	OS 1201544	1,2,3,6,7,8-HxCDF	4
69	LUFA-Prüfbericht LV4-RU-0008-2012	0		Styropor	113	0,2	OS 1201544	1,2,3,7,8,9-HxCDF	4
69	LUFA-Prüfbericht LV4-RU-0008-2012	0		Styropor	114	0,2	OS 1201544	2,3,4,6,7,8-HxCDF	4
69	LUFA-Prüfbericht LV4-RU-0008-2012	0,55		Styropor	115	0	OS 1201544	1,2,3,4,6,7,8-HpCDF	4
69	LUFA-Prüfbericht LV4-RU-0008-2012	0		Styropor	116	0,5	OS 1201544	1,2,3,4,7,8,9-HpCDF	4
69	LUFA-Prüfbericht LV4-RU-0008-2012	0		Styropor	117	5	OS 1201544	OCDF	4

Figure 33: Output format for sample analyses

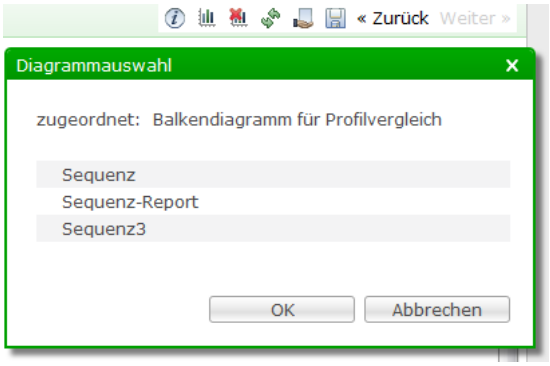


Figure 34: Selection of a sample analysis

In the last tab, “Graphic view”, the results can be shown in a diagram (select:). The bar chart suitable for the profile comparison can be applied to the results set with or without analysis. In addition to the contaminated sample, the most similar sample is shown, plus all source profiles selected in Fig. 5 (Fig. 11).

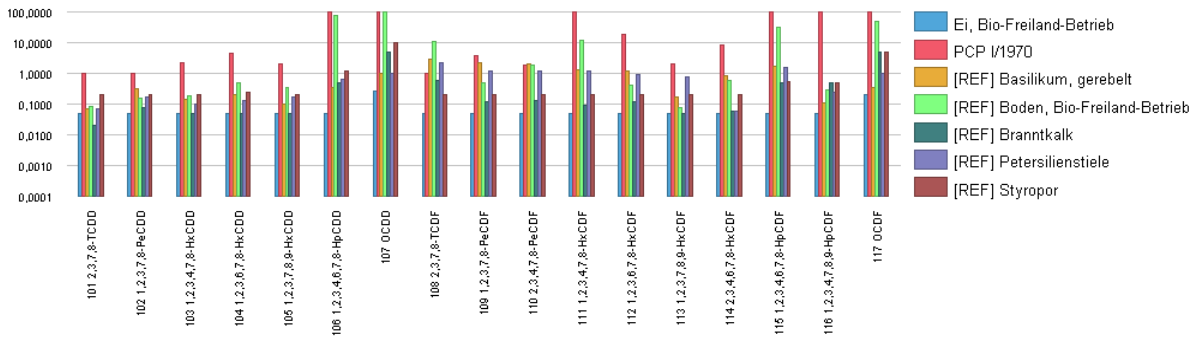


Figure 35: Bar chart of results set